Materials Design for Superconductors

Michael Norman

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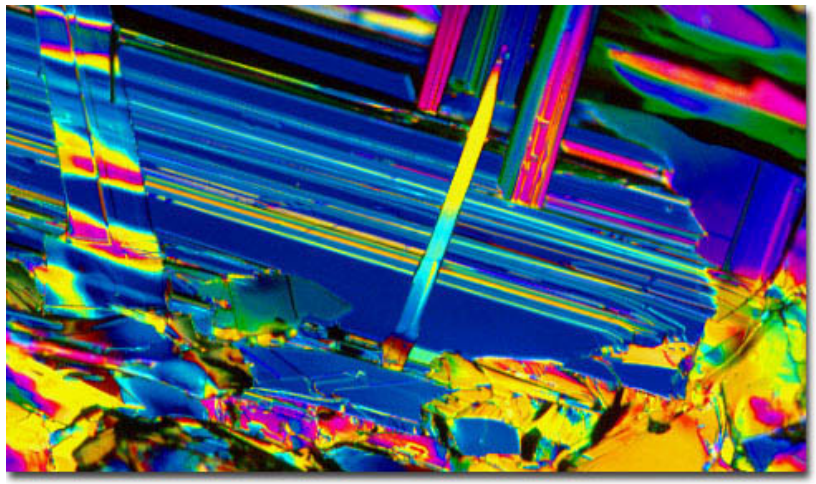
&
Center for Emergent Superconductivity
Argonne National Laboratory



NWU – Jan 14, 2014

Materials Genome Initiative
for Global Competitiveness

June 2011

To help businesses discover, develop, and deploy new materials twice as fast, we're launching what we call ***the Materials Genome Initiative****. The invention of silicon circuits and lithium ion batteries made computers and iPods and iPads possible, but it took years to get those technologies from the drawing board to the market place. We can do it faster.*

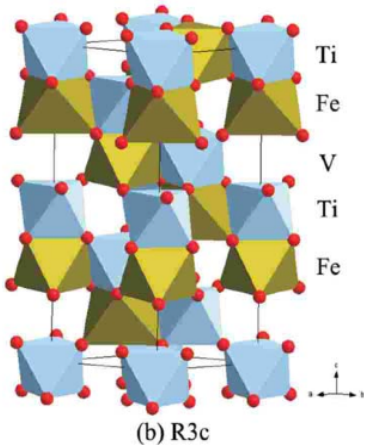
-President Obama
Carnegie Mellon University, June 2011

“Multiferroic By Design”

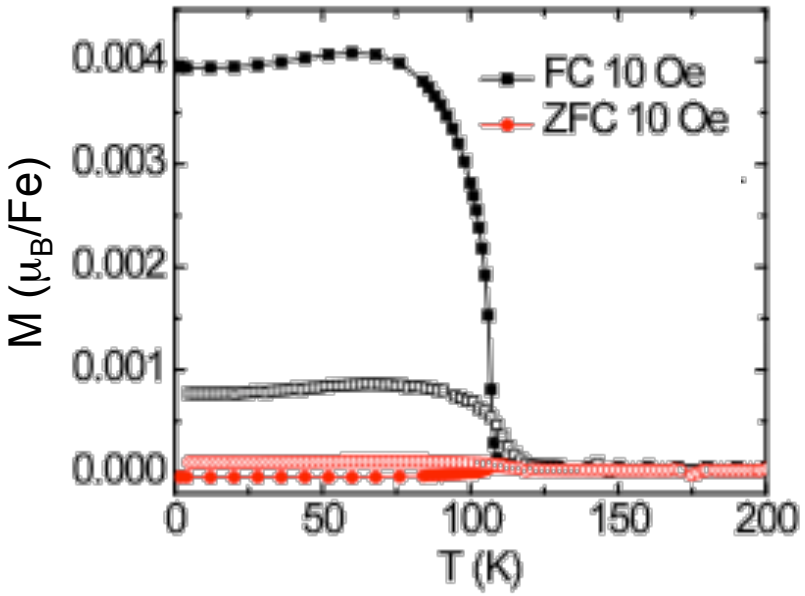
High pressure form of $FeTiO_3$

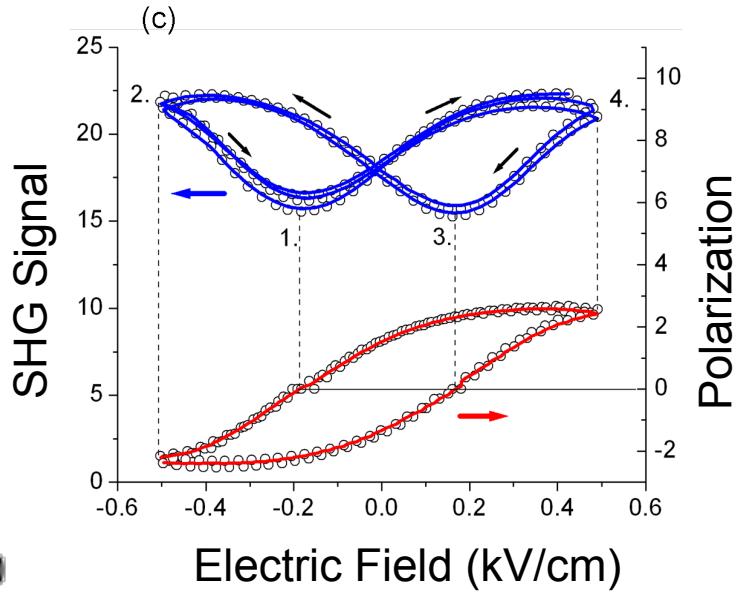
Predicted by Craig Fennie

Synthesized by John Mitchell’s group



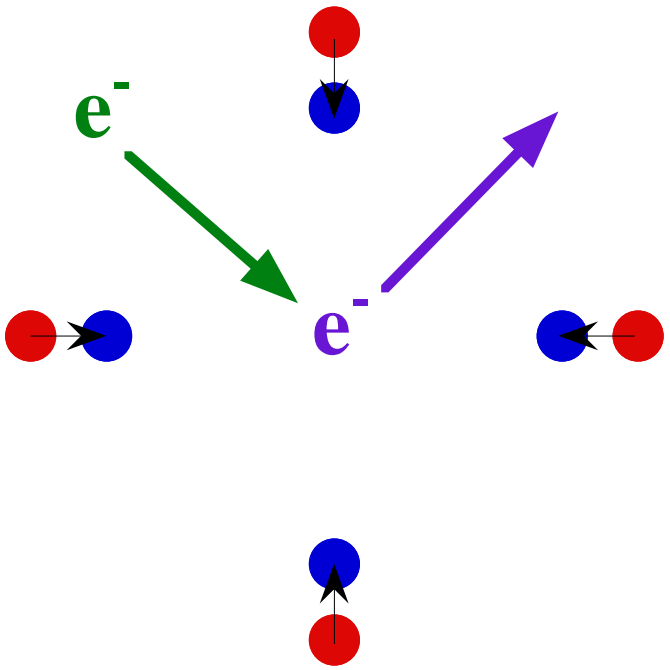
(b) R3c





Varga *et al.*, PRL 103, 047601 (2009)

Predicting ferroelectrics is one thing, but superconductors is quite another. Even conventional superconductors involve a subtle interplay of electron-ion and electron-electron interactions.

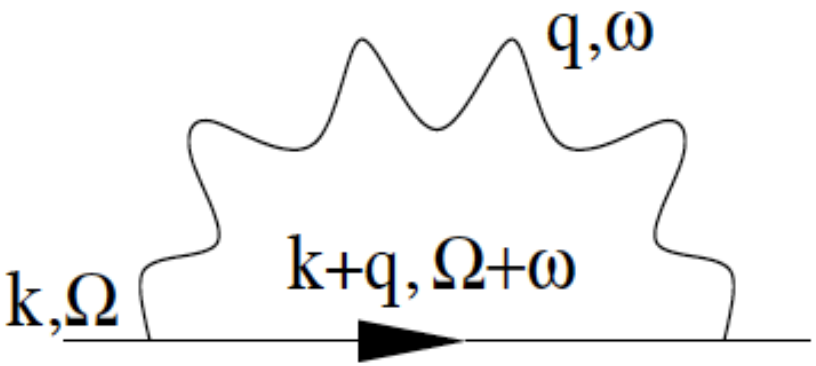


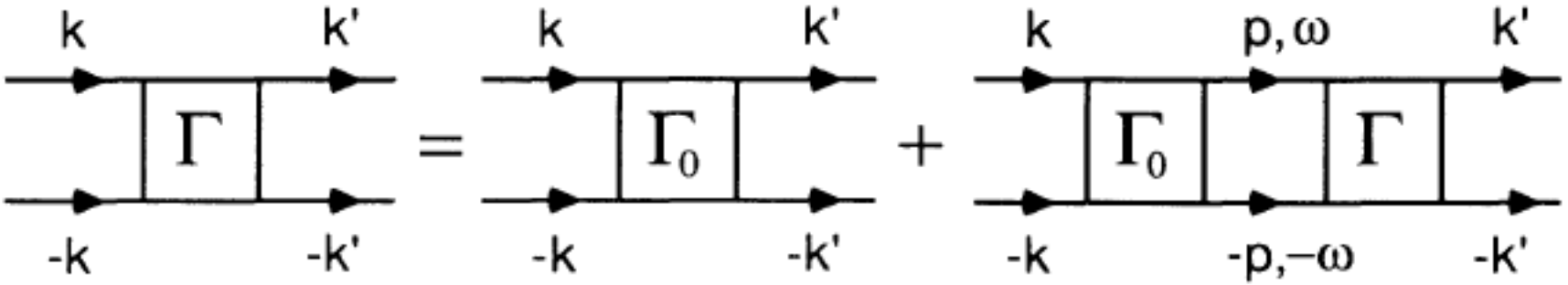
1. 1st e^- attracts + ions
2. Ions shift position from red to blue
3. 1st e^- moves away
4. 2nd e^- sees + ion hole and moves to former position of 1st e^-

Interaction is local in space
(s-wave pairs, L=0, S=0)
but retarded in time
(T_c << Debye frequency)

$$T_c \sim \omega_D \, e^{-1/(\lambda - \mu^*)}$$

In conventional electron-phonon theory, we rapidly went from a weak coupling treatment – BCS - to a strong coupling theory – Eliashberg - in just a few years because of the utility of Migdal's theorem

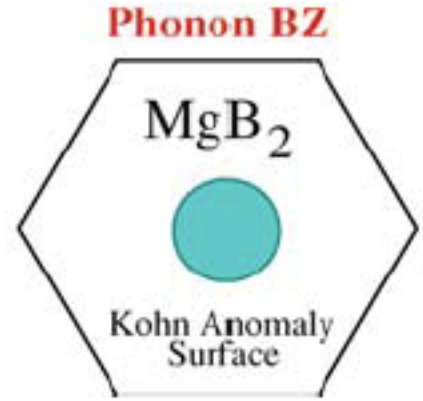


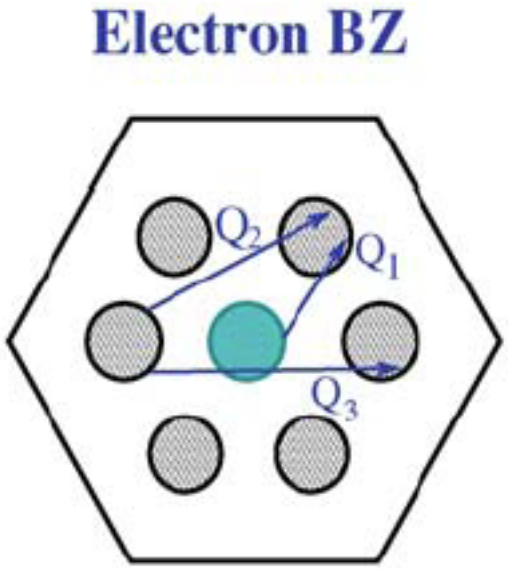


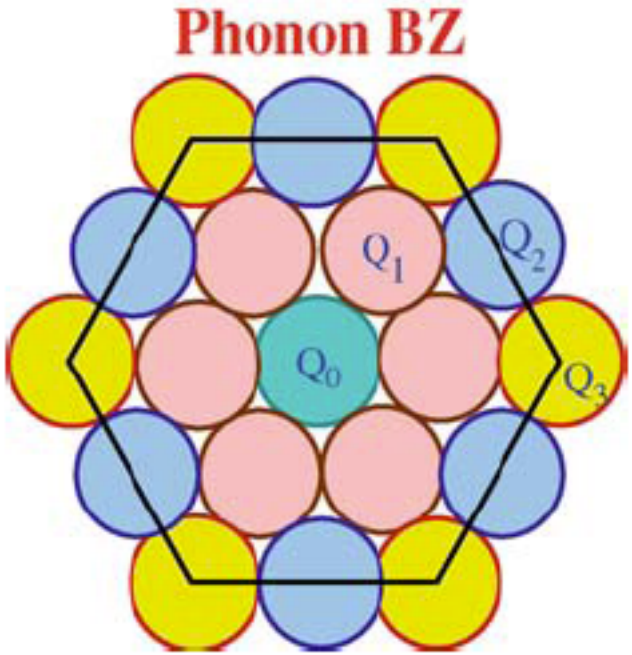
Unfortunately, this didn't help us much!

1. Didn't predict buckeyballs
2. Didn't predict MgB_2
3. Predictions based on MgB_2 (Li_xBC, etc.) didn't pan out
4. Heavy fermion superconductors unexpected
5. Cuprates as well
6. Pnictides too
7. And we can only imagine what's next …

Rational design for new HTS – select band structure to enable phonons to use more of the BZ







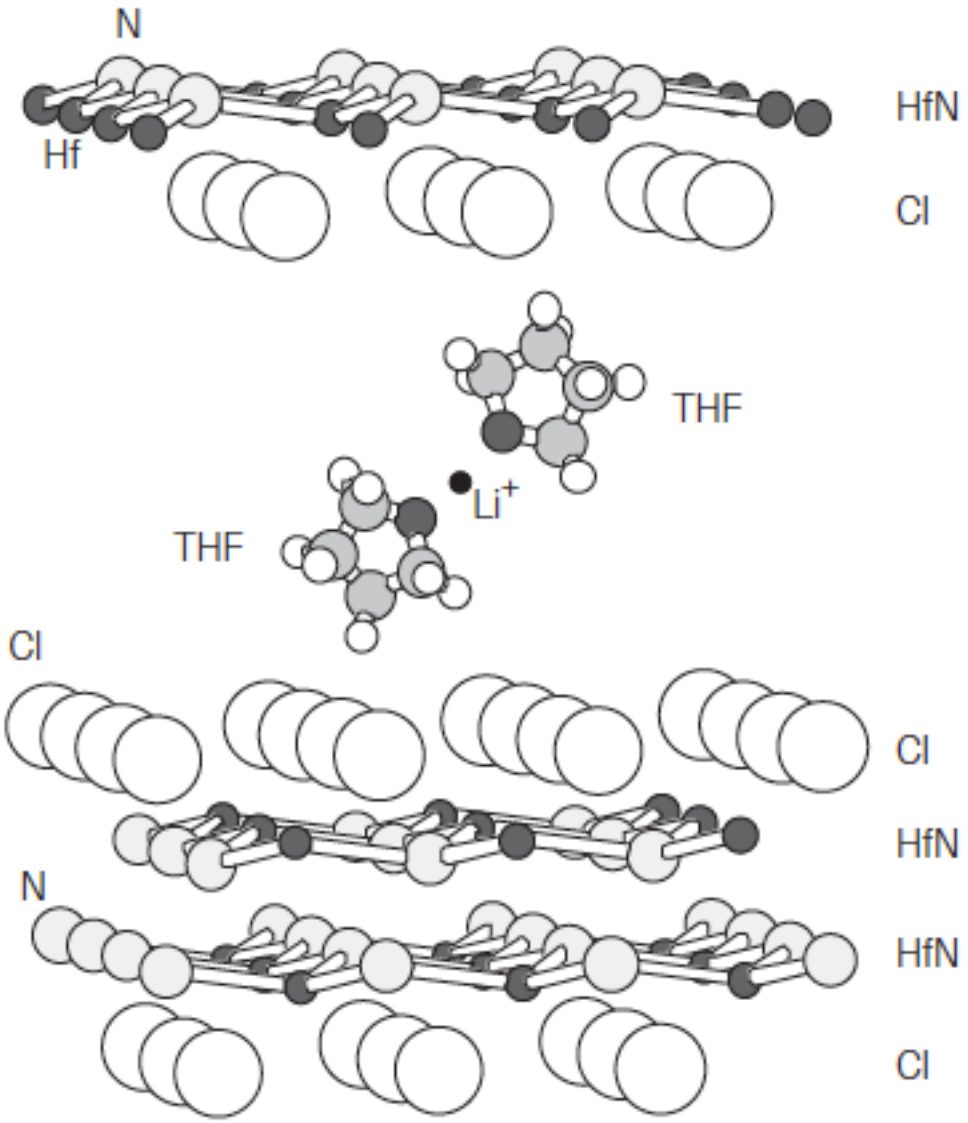
Pickett, J Superconductivity 19, 291 (2006)

Rules of B. Matthias for discovering new superconductors

1. high symmetry is best
2. peaks in density of states are good
3. stay away from oxygen
4. stay away from magnetism
5. stay away from insulators
6. stay away from theorists

From Steve Girvin's lecture (Boulder Summer School 2000) courtesy of Matthew Fisher

26K superconductivity in layered hafnium nitride (a doped ionic insulator)



Yamanaka *et al.*, Nature (1998)

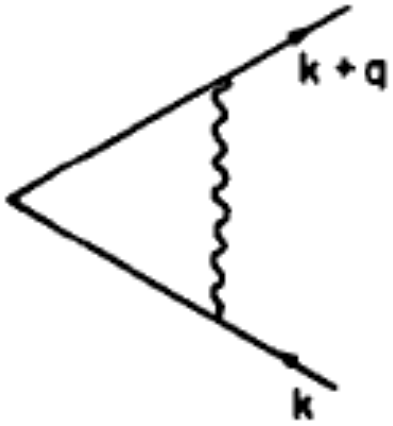
So, what do we mean by unconventional superconductivity?

1. An order parameter that changes sign as a function of momentum

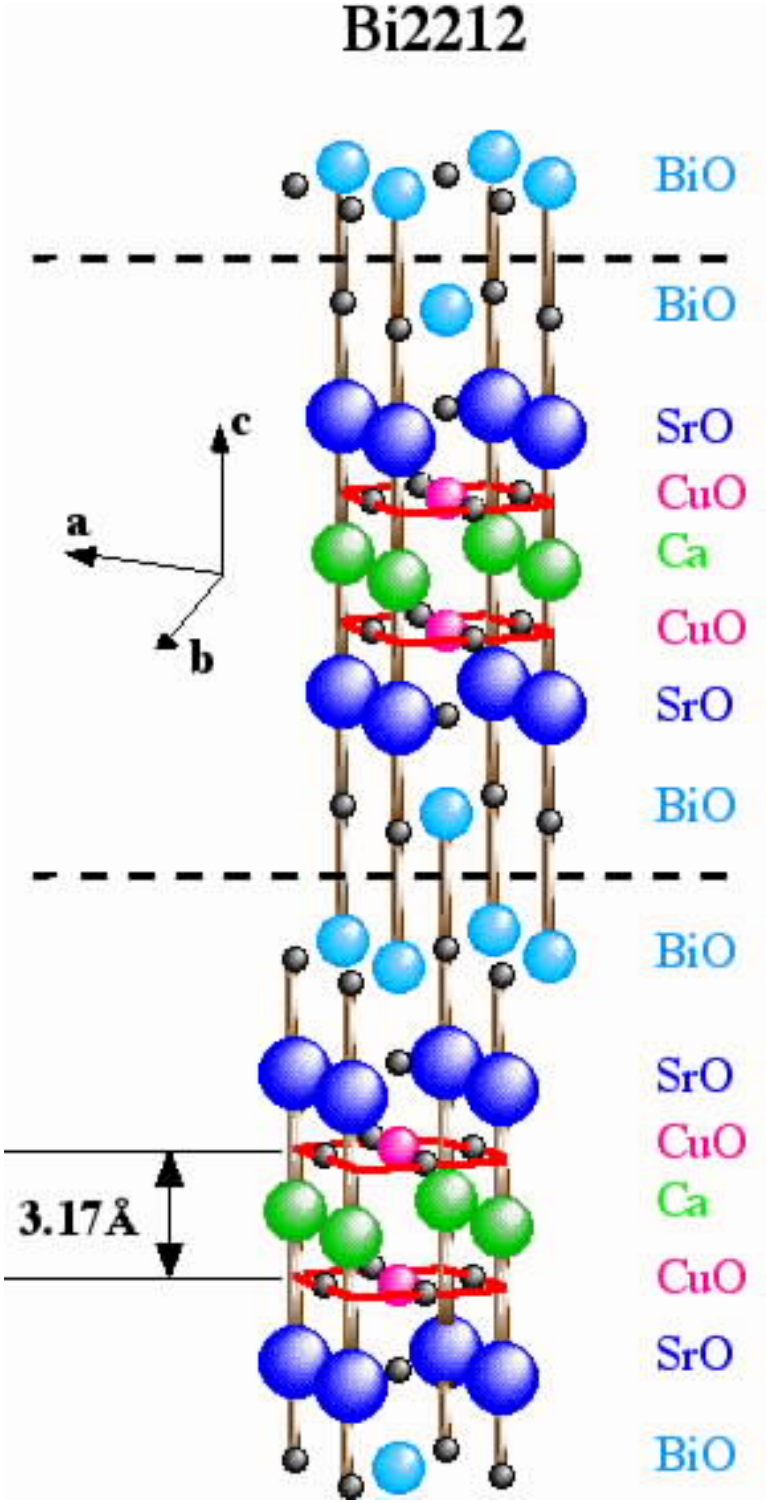
2. A pairing mechanism different from electron-phonon theory

Examples

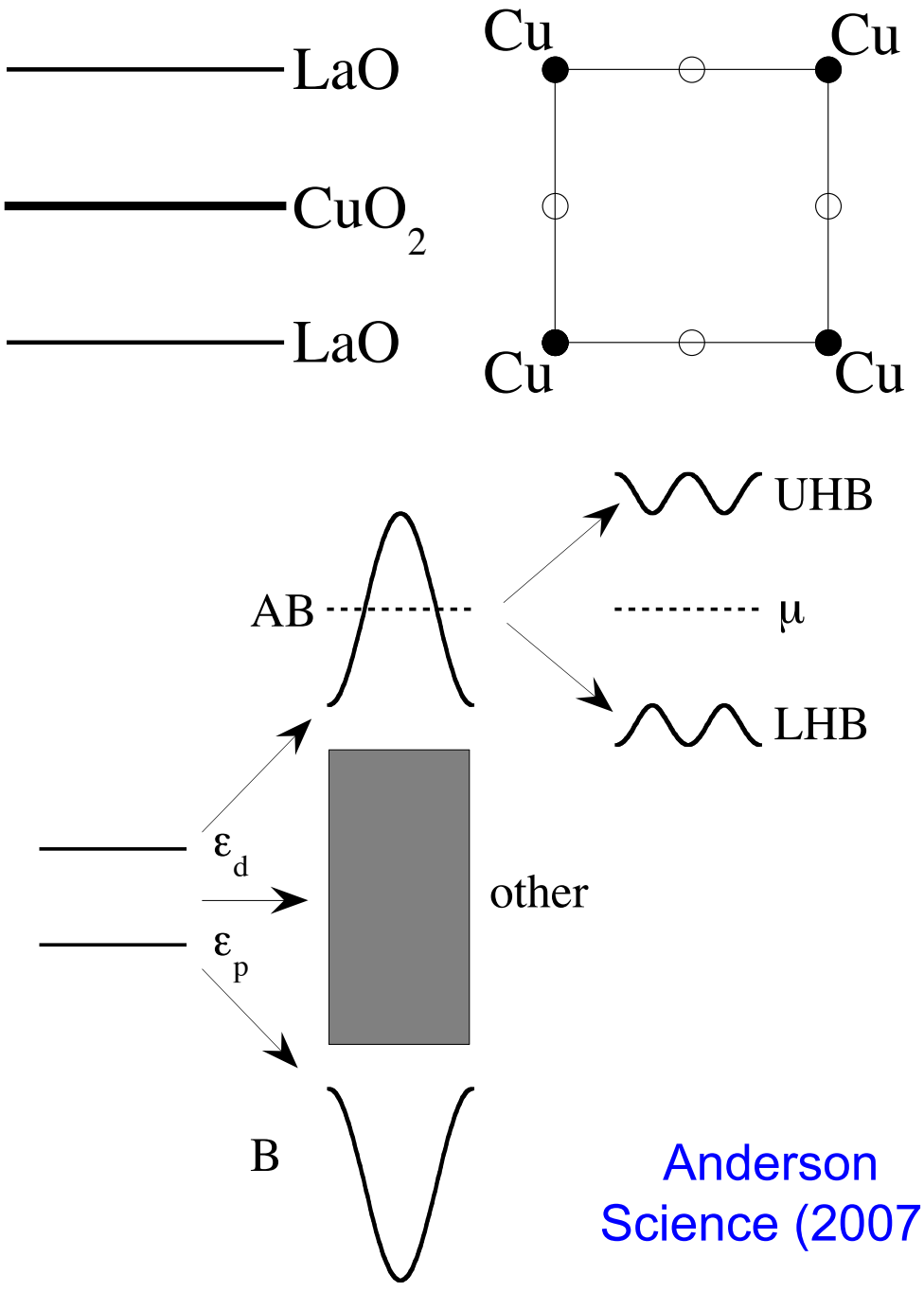
- superfluid ^{3}He
- heavy fermion superconductors
- organic superconductors
- cuprate superconductors
- iron arsenide superconductors



As pointed out by Hertz, Levin and Beal-Monod (SSC 1976), there is no Migdal's theorem for electron-electron theories



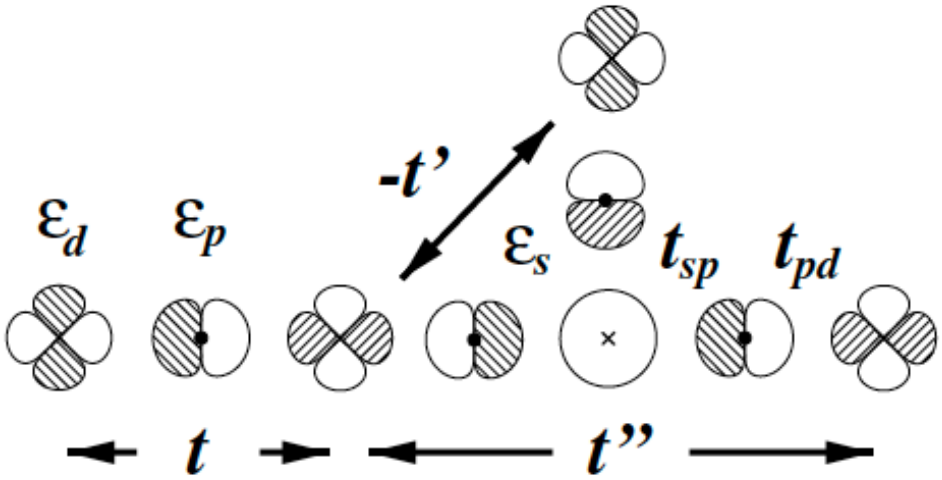
Electronic Structure of Cuprates

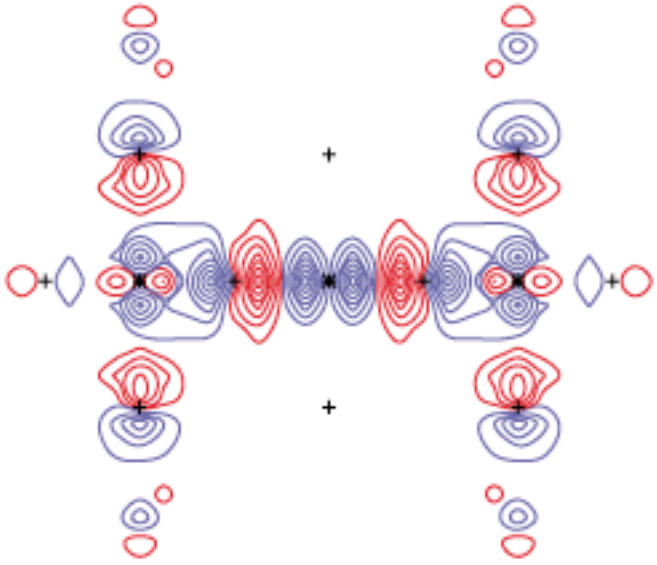


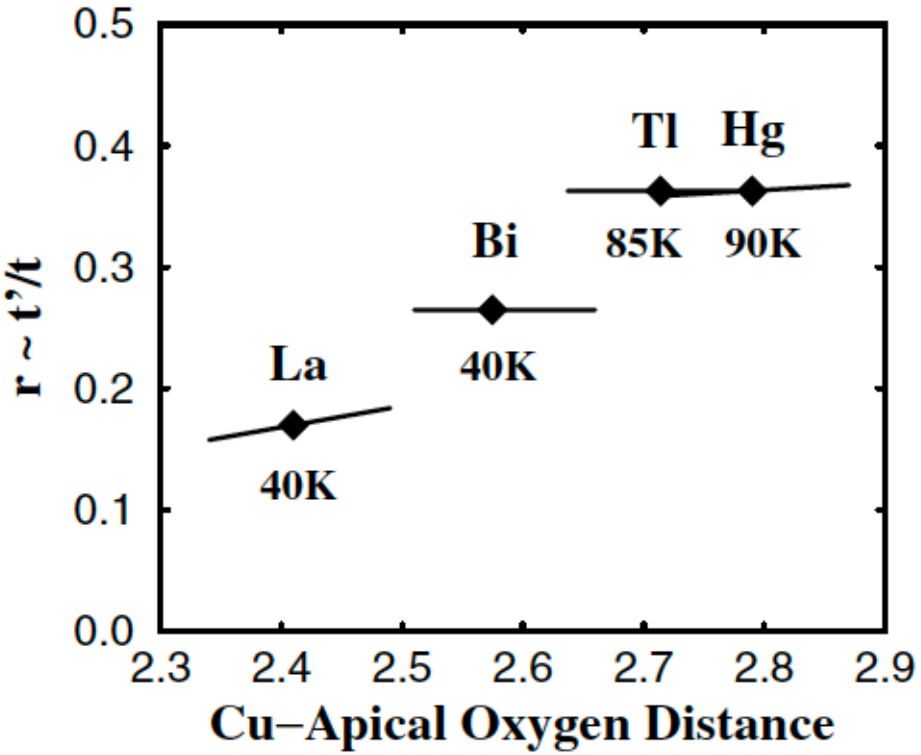
Anderson
Science (2007)

Band-Structure Trend in Hole-Doped Cuprates and Correlation with $T_{c\,max}$

E. Pavarini, I. Dasgupta,* T. Saha-Dasgupta,† O. Jepsen, and O. K. Andersen

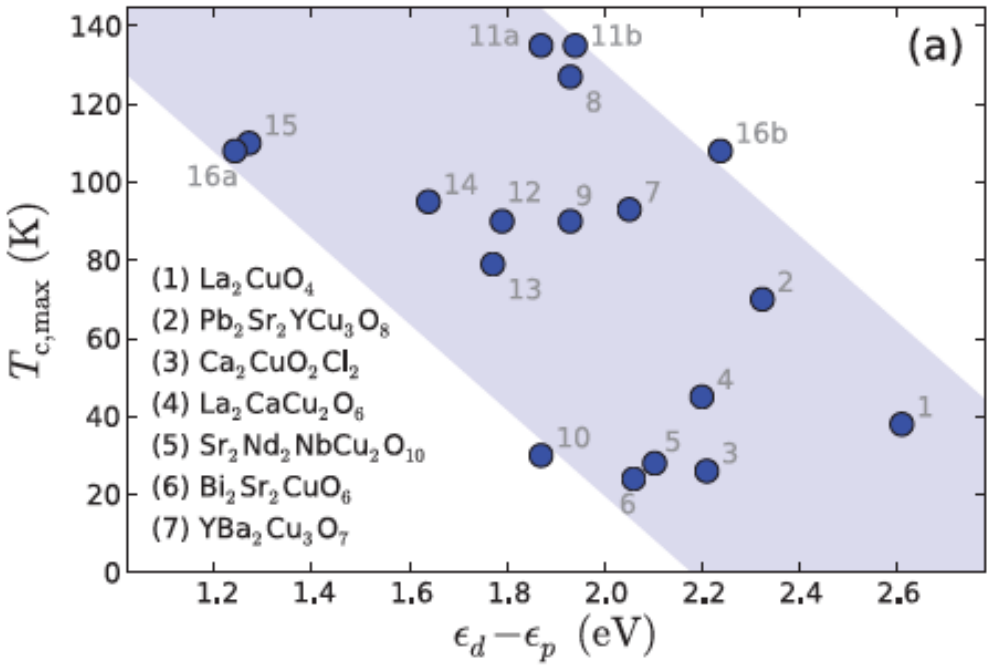


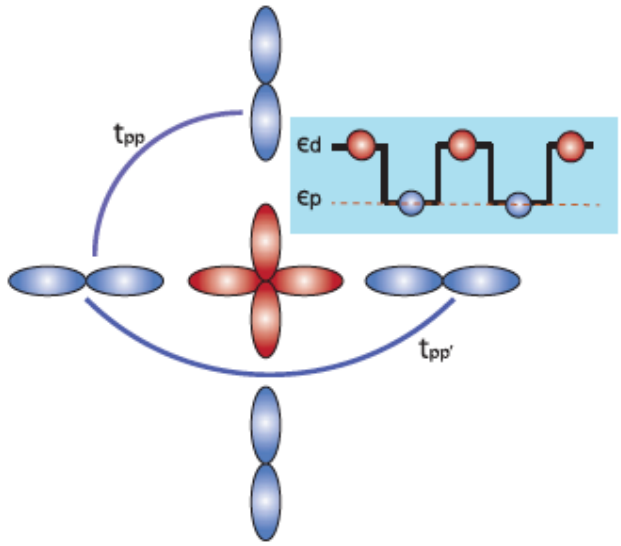


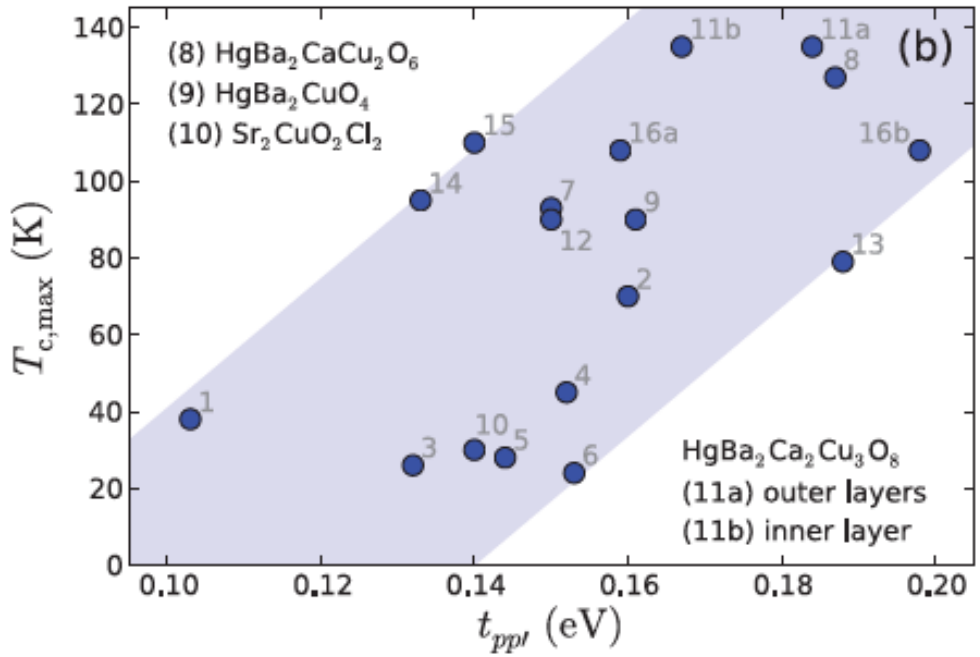


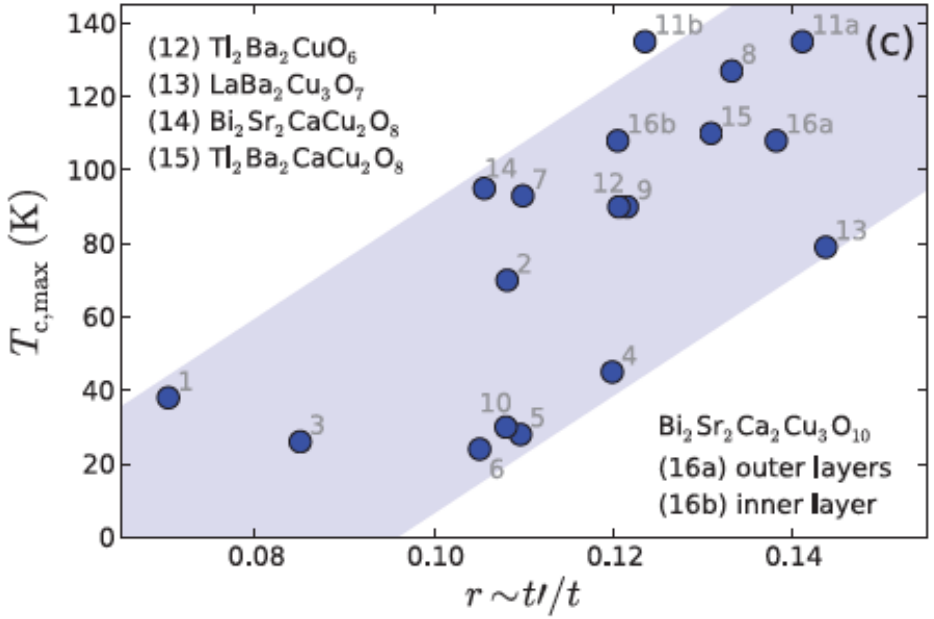
Pavarini *et al*, PRL 87, 047003 (2001)

Cluster Dynamical Mean Field Theory



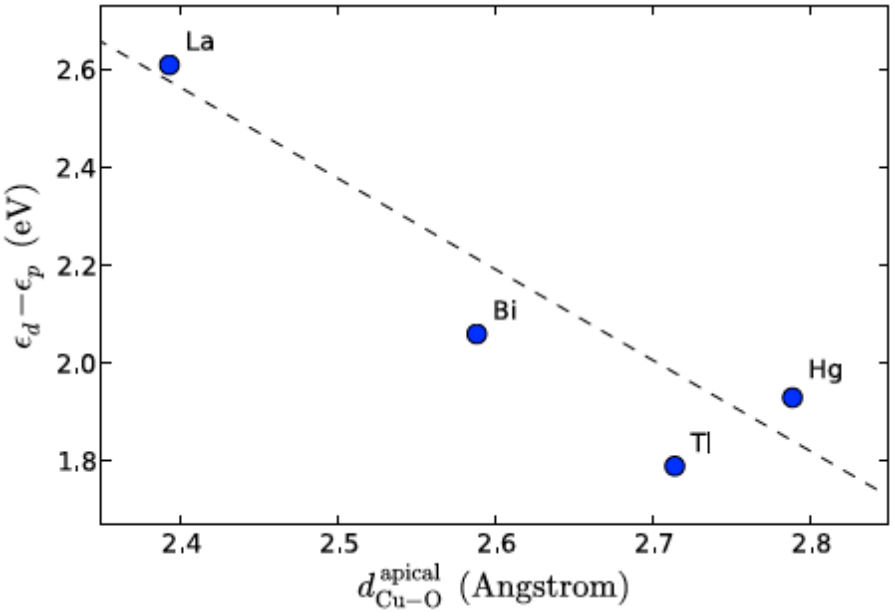


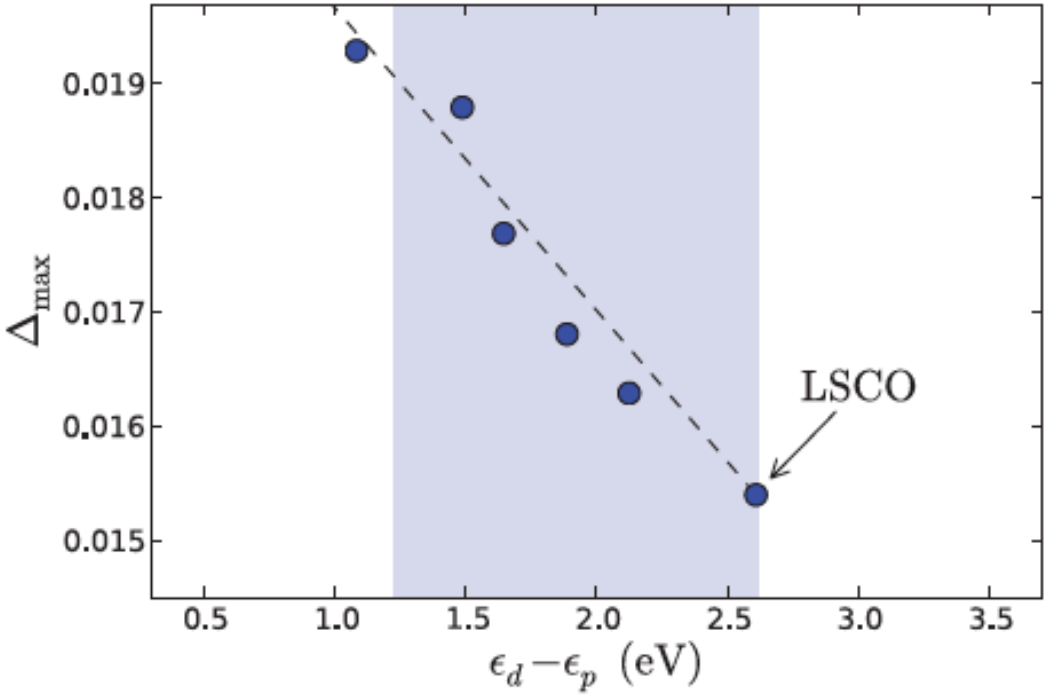


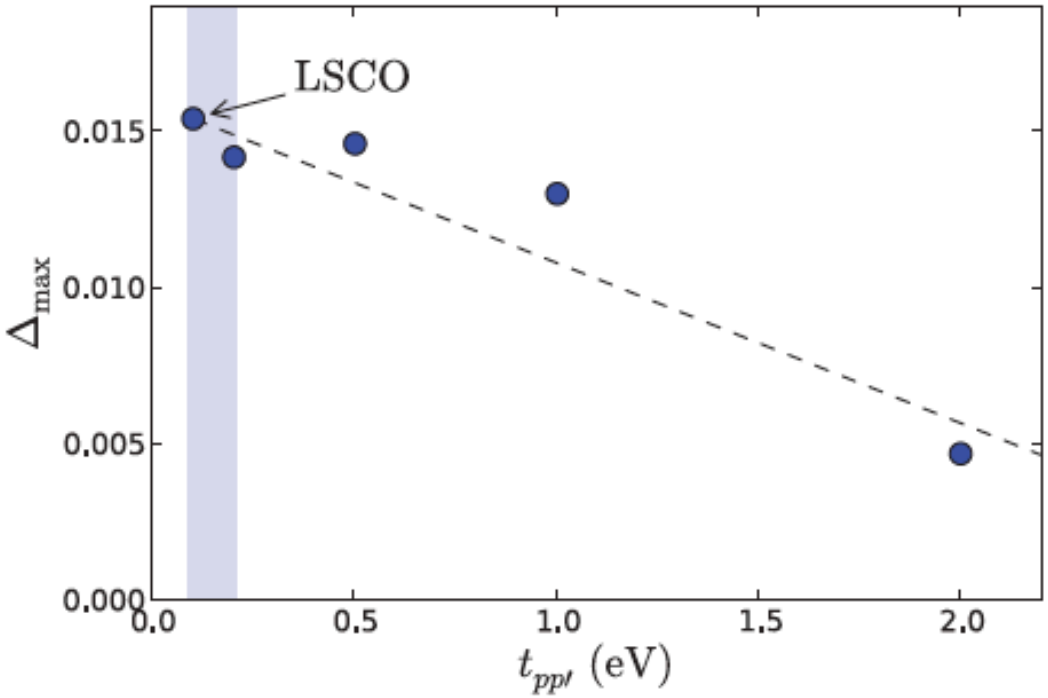


Weber *et al.*, EPL 100, 37001 (2012)

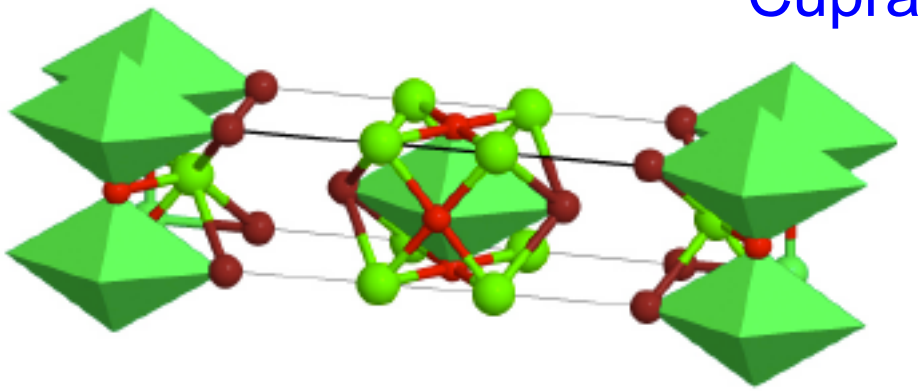
T_c vs ε_p-ε_d



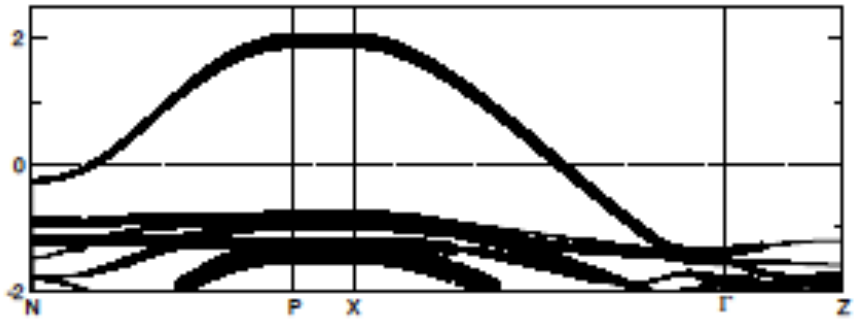


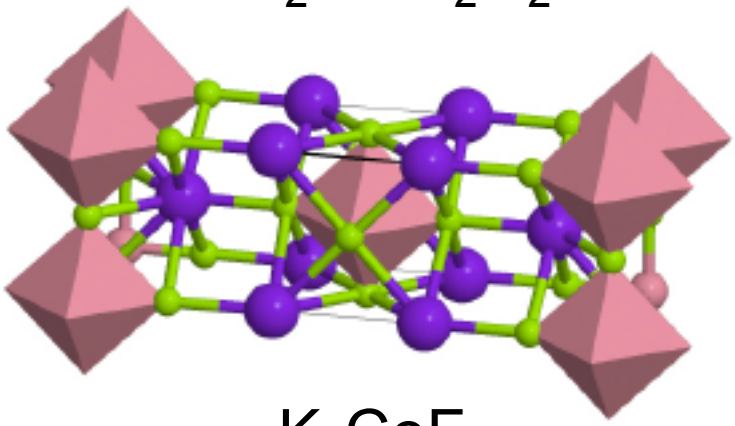


Data Mining (over 60,000 electronic structures)
Cuprate analogues?

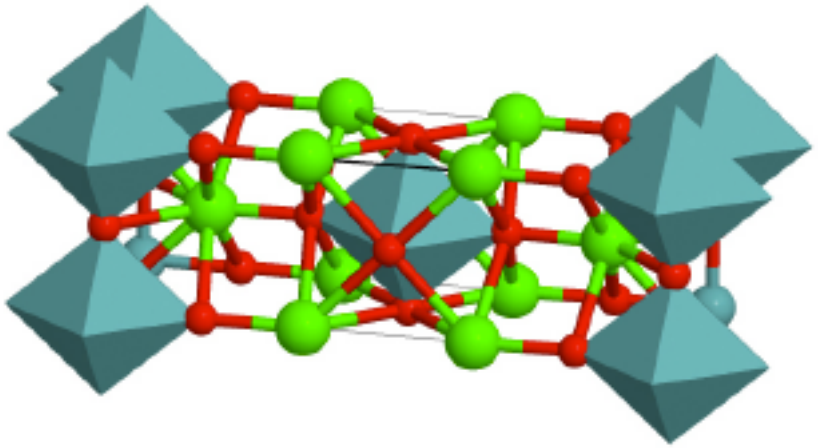


$Ca_2CuBr_2O_2$

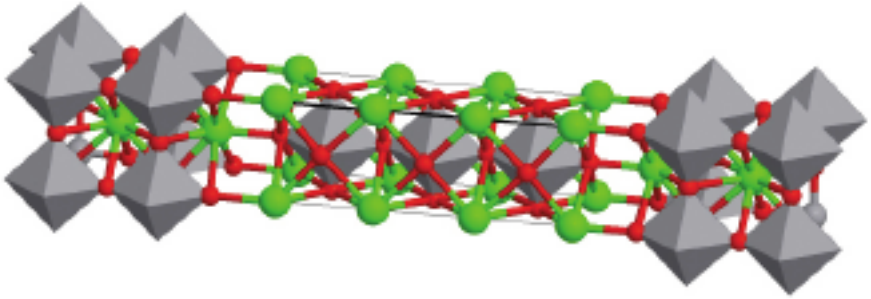




K_2CoF_4



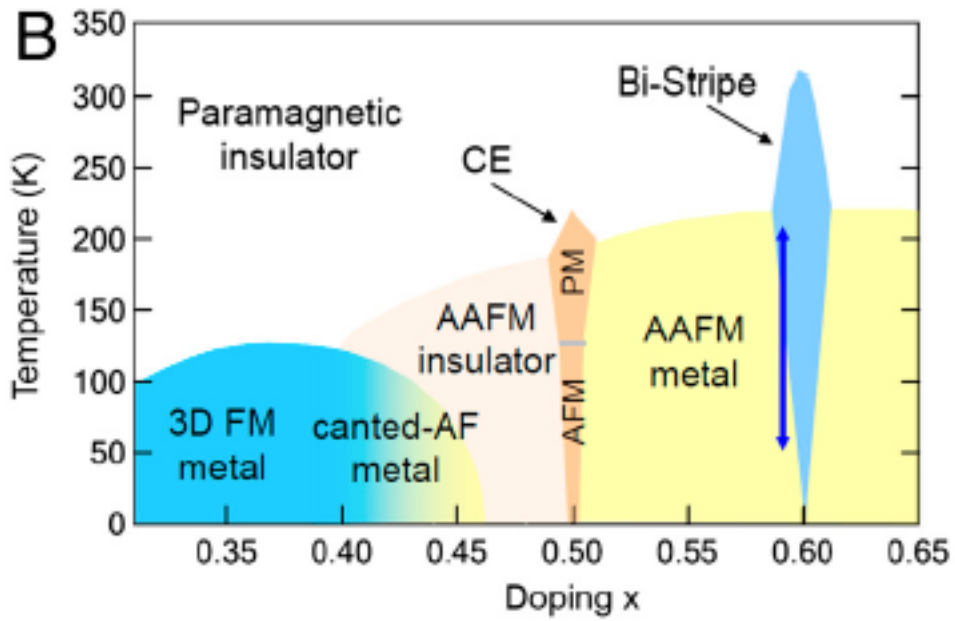
Sr_2MoO_4

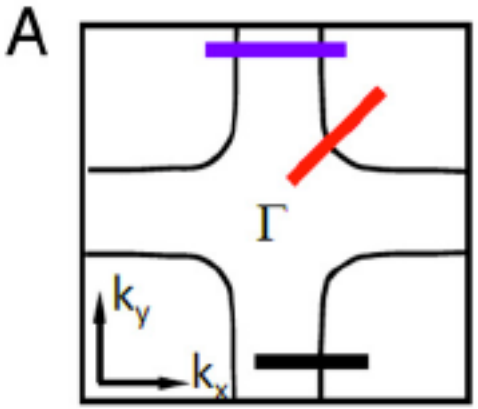


$Sr_4V_3O_{10}$

Klintenberg & Eriksson, Comp Matls Sci 67, 282 (2013)

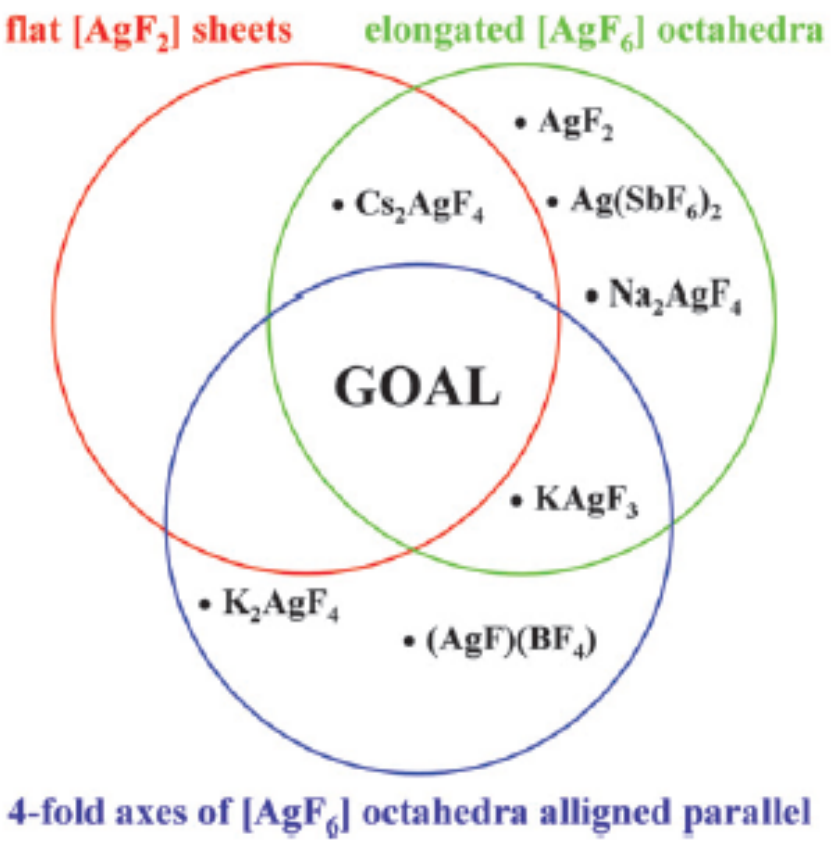
But manganites have similar electronic properties as cuprates
- i.e., a large hole Fermi surface centered around (π,π) –
yet are ferromagnets, not superconductors

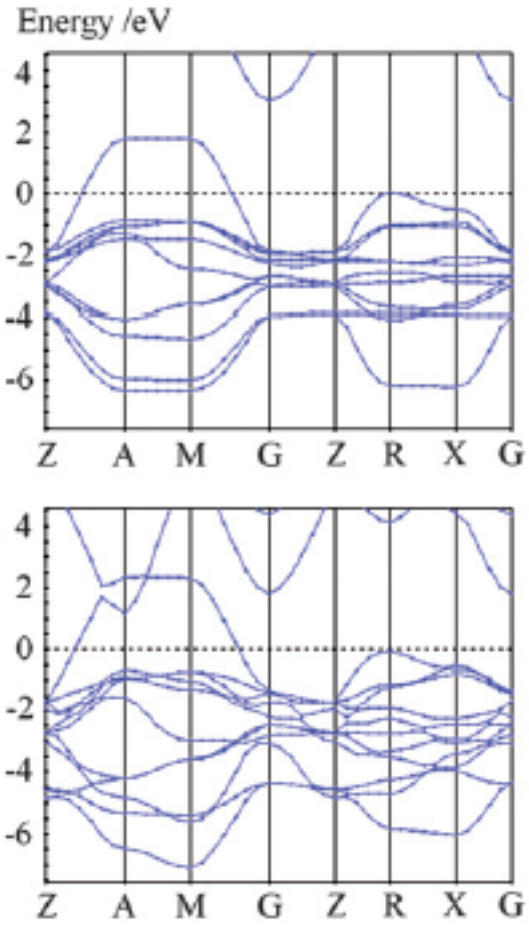


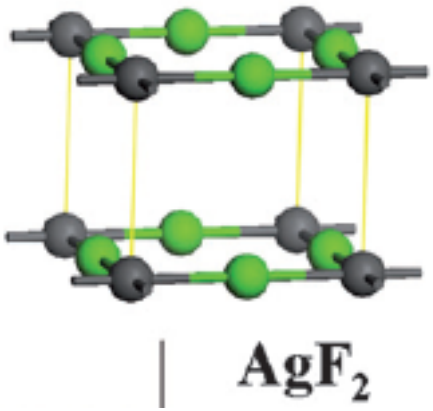


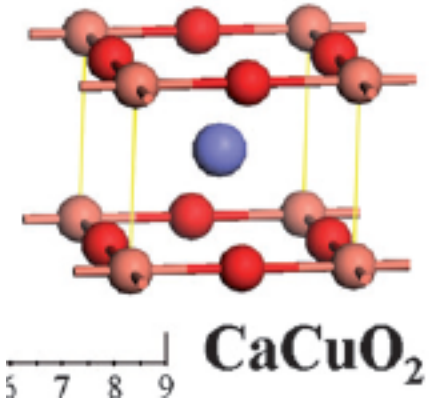
Sun *et al.*, PNAS (2011)

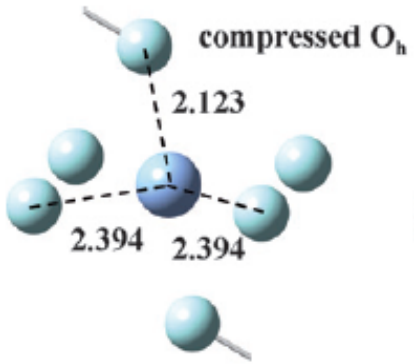
Quantum Chemical Considerations – Silver Flourides









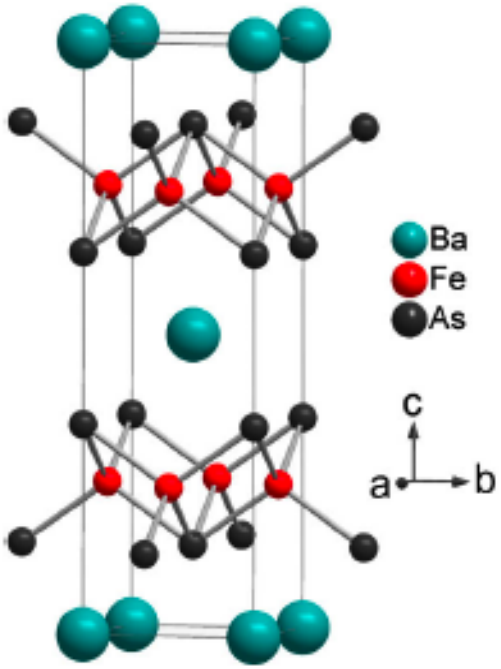


$Ag(BF_4)_2(FH)_4$

Grochala, J. Mater. Chem.19, 6949 (2009)

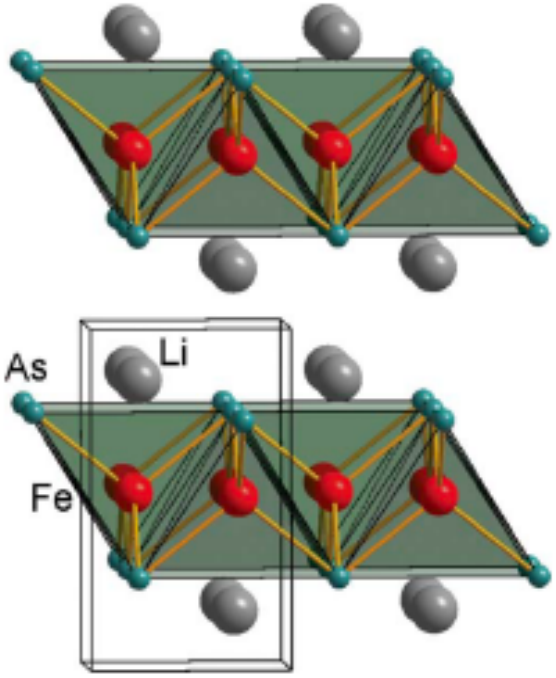
Iron arsenide and chalcogenide superconductors
There are a number of different crystal structures

122



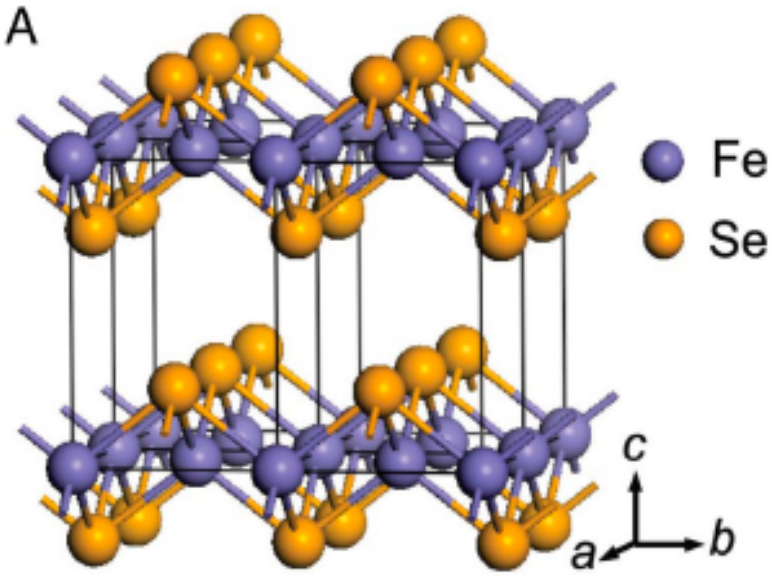
Rotter *et al.*, PRL (2008)

111



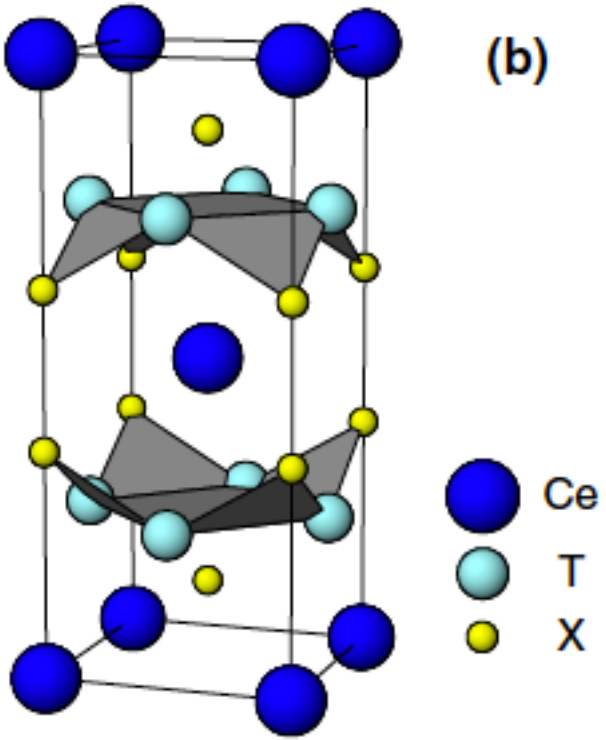
Tapp *et al.*, PRB (2008)

11

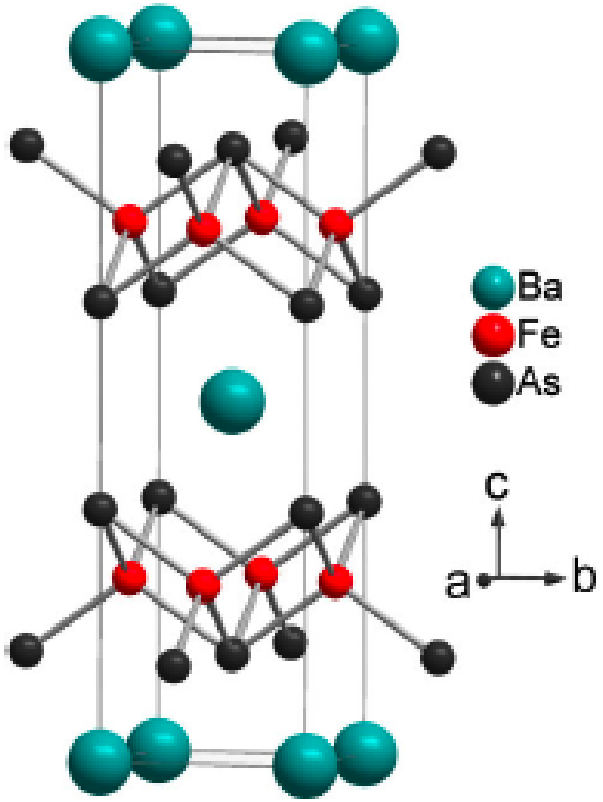


Hsu *et al.*, PNAS (2008)

$ThCr_2Si_2$ crystal structure seems to be ubiquitous ($CeCu_2Si_2$ is a heavy fermion superconductor)

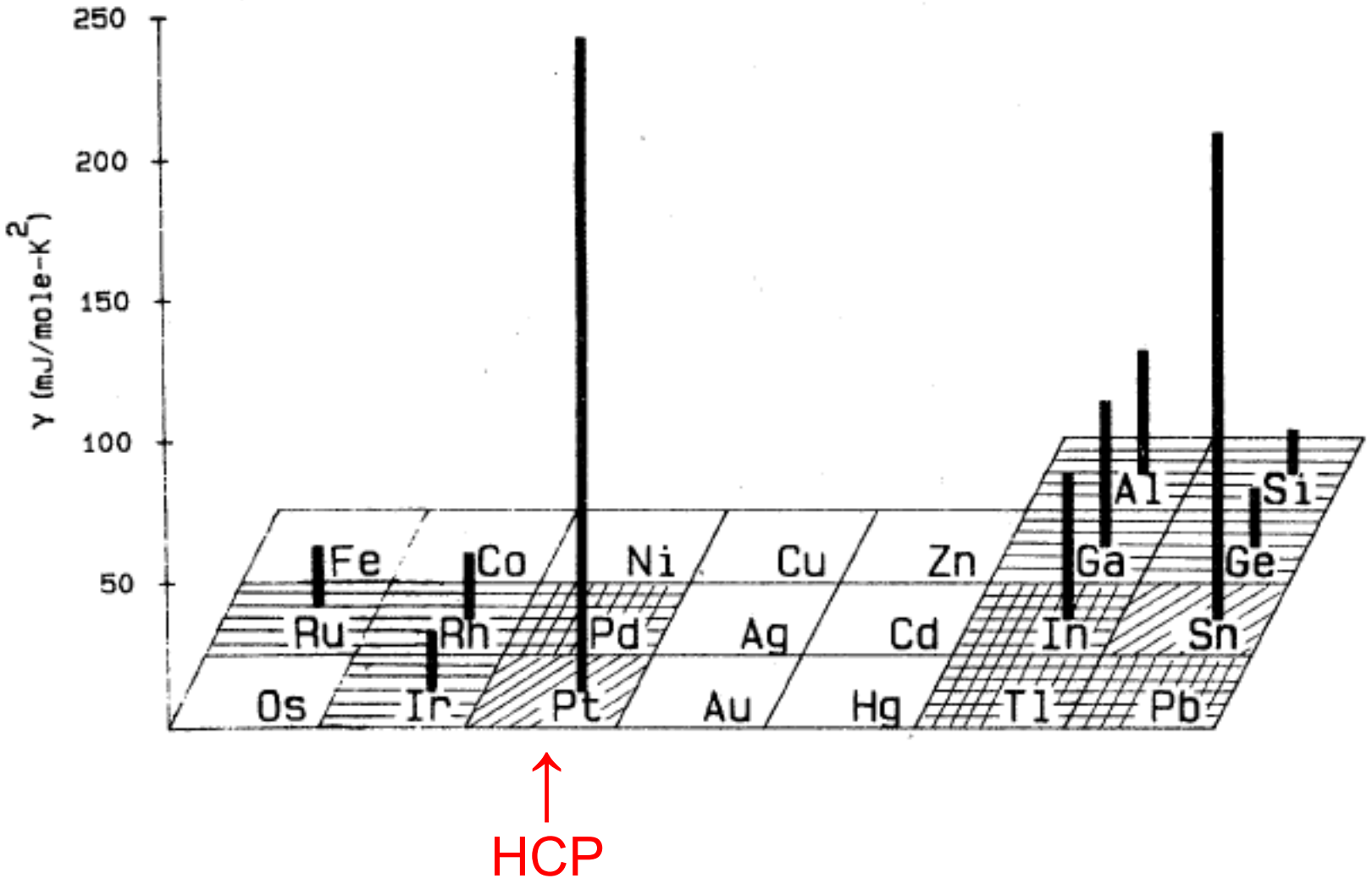


$CeCu_2Si_2$



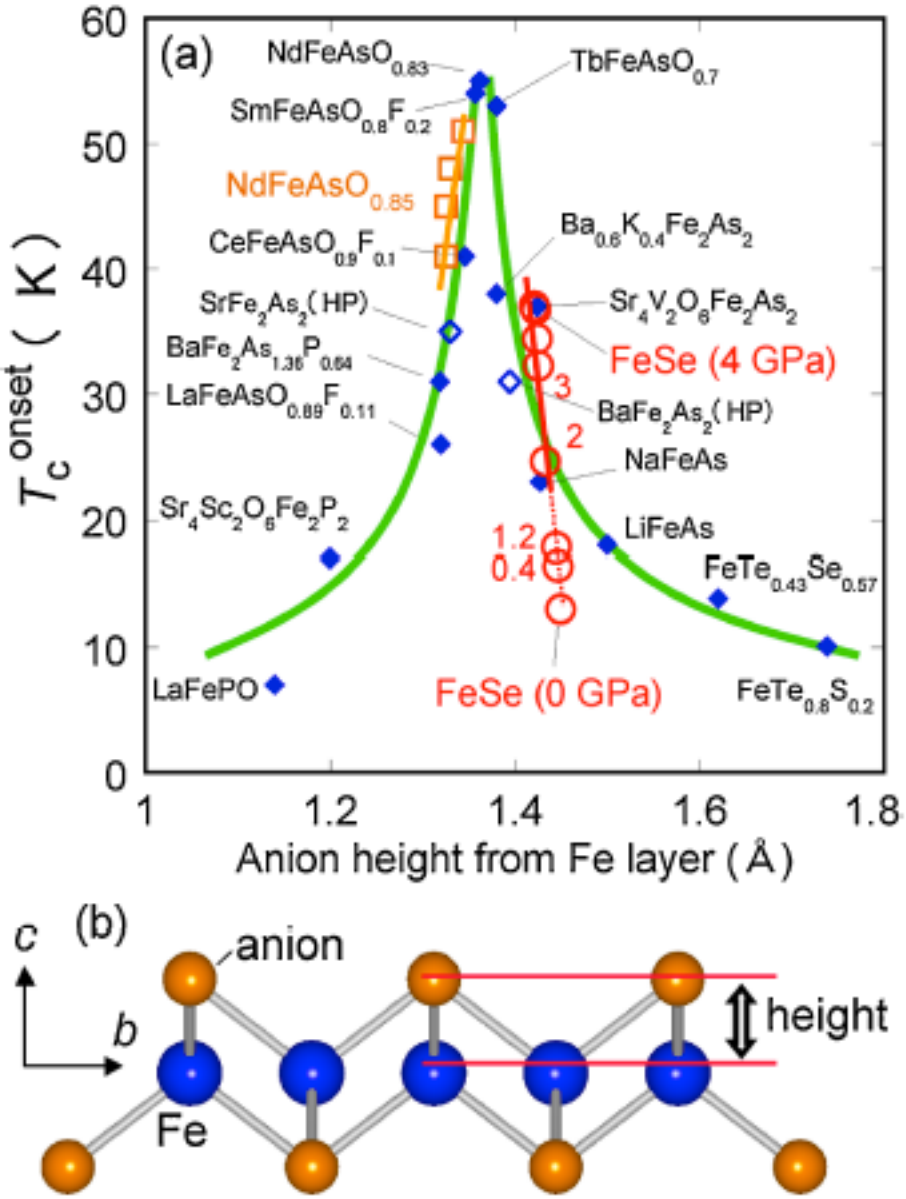
$BaFe_2As_2$

UX_3 – most of them $AuCu_3$ cubic structure except
UPd_3 – dHCP (localized f electrons, quadrupole order)
UPt_3 – HCP (itinerant f, heavy fermion superconductor)



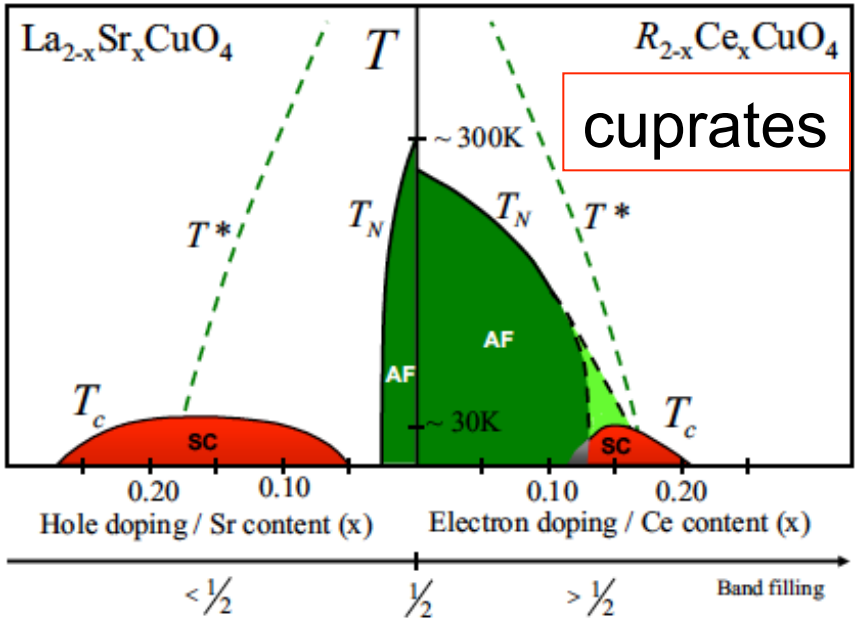
Koelling *et al.*, PRB (1985)

Tuning T_c in iron pnictides/chalcogenides via anion height

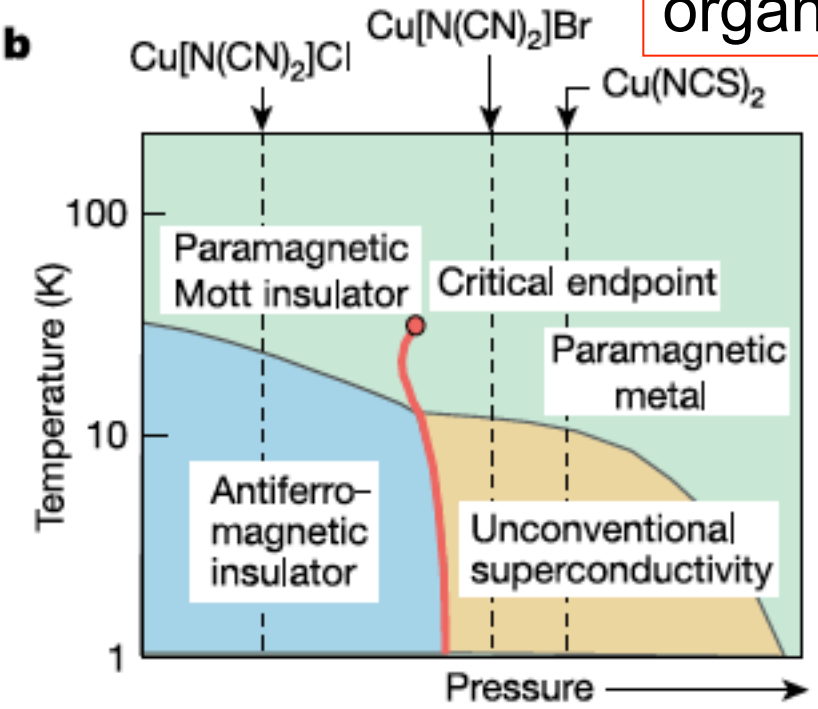


Mizuguchi & Takano, JPSJ 79, 102001 (2010)

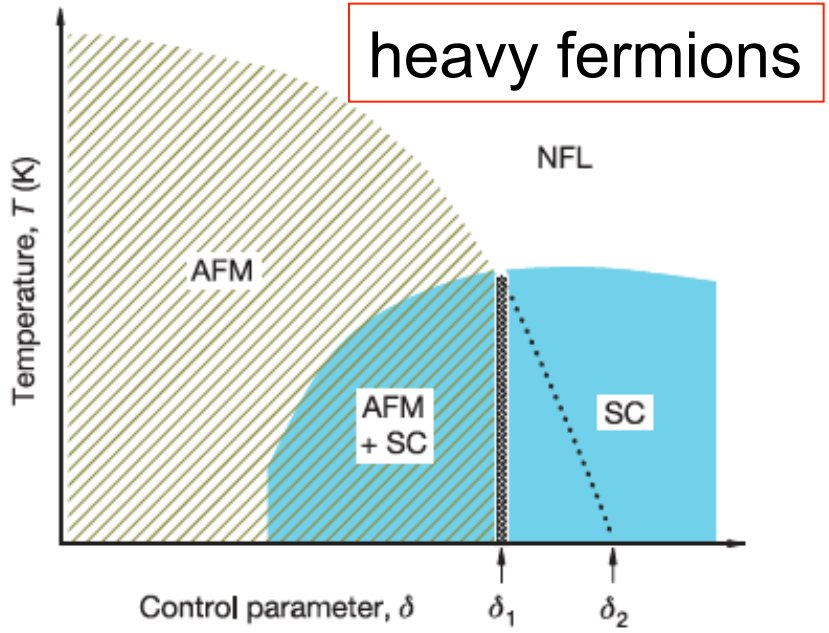
Similarity of Phase Diagrams



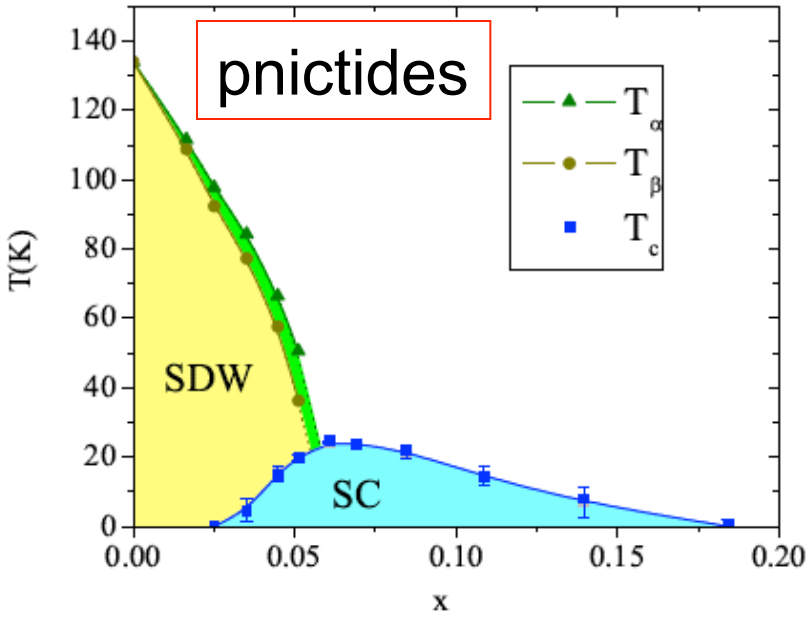
organics



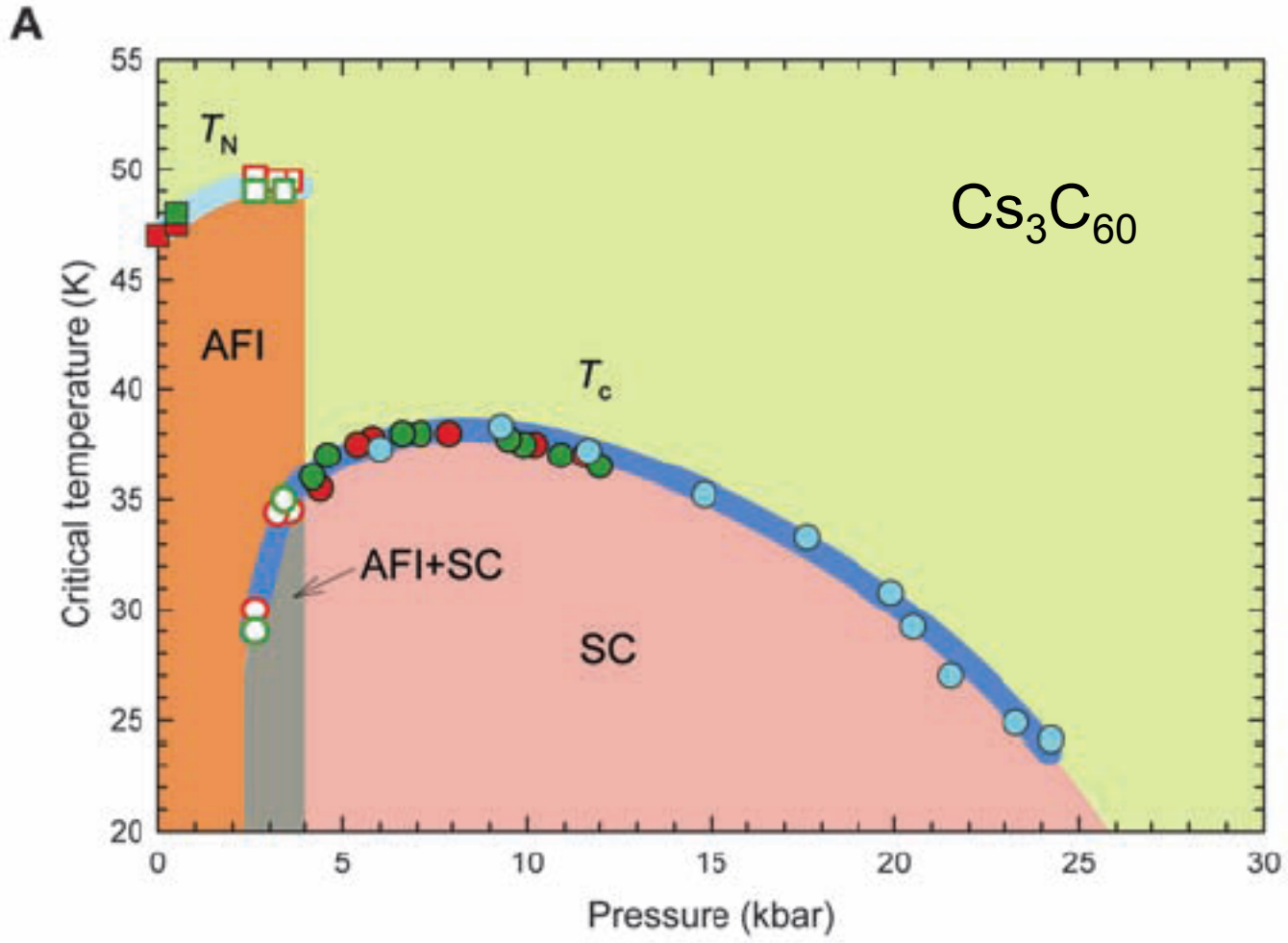
heavy fermions



pnictides

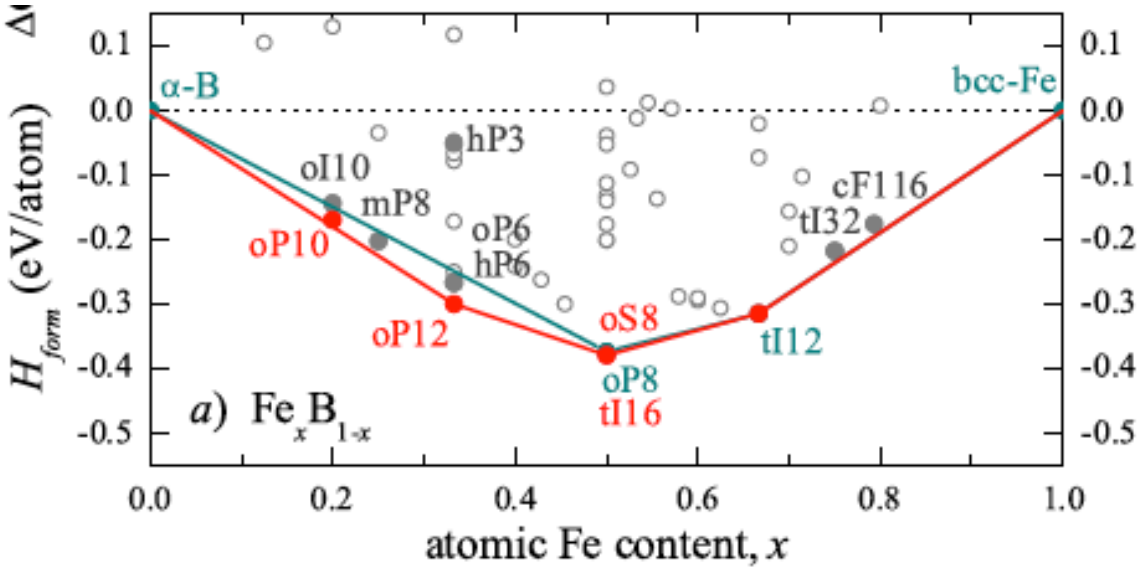


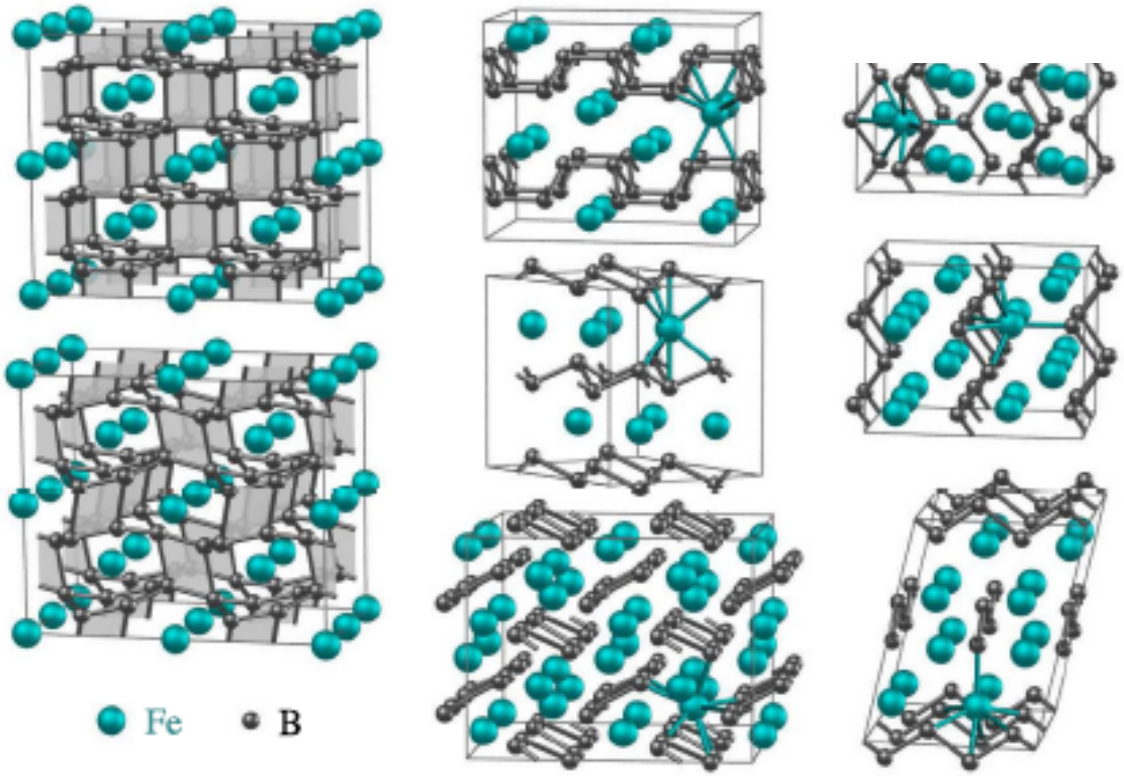
Even Buckeyballs have a Similar Phase Diagram



Takabayashi *et al*., Science (2009)

Evolutionary Search - FeB





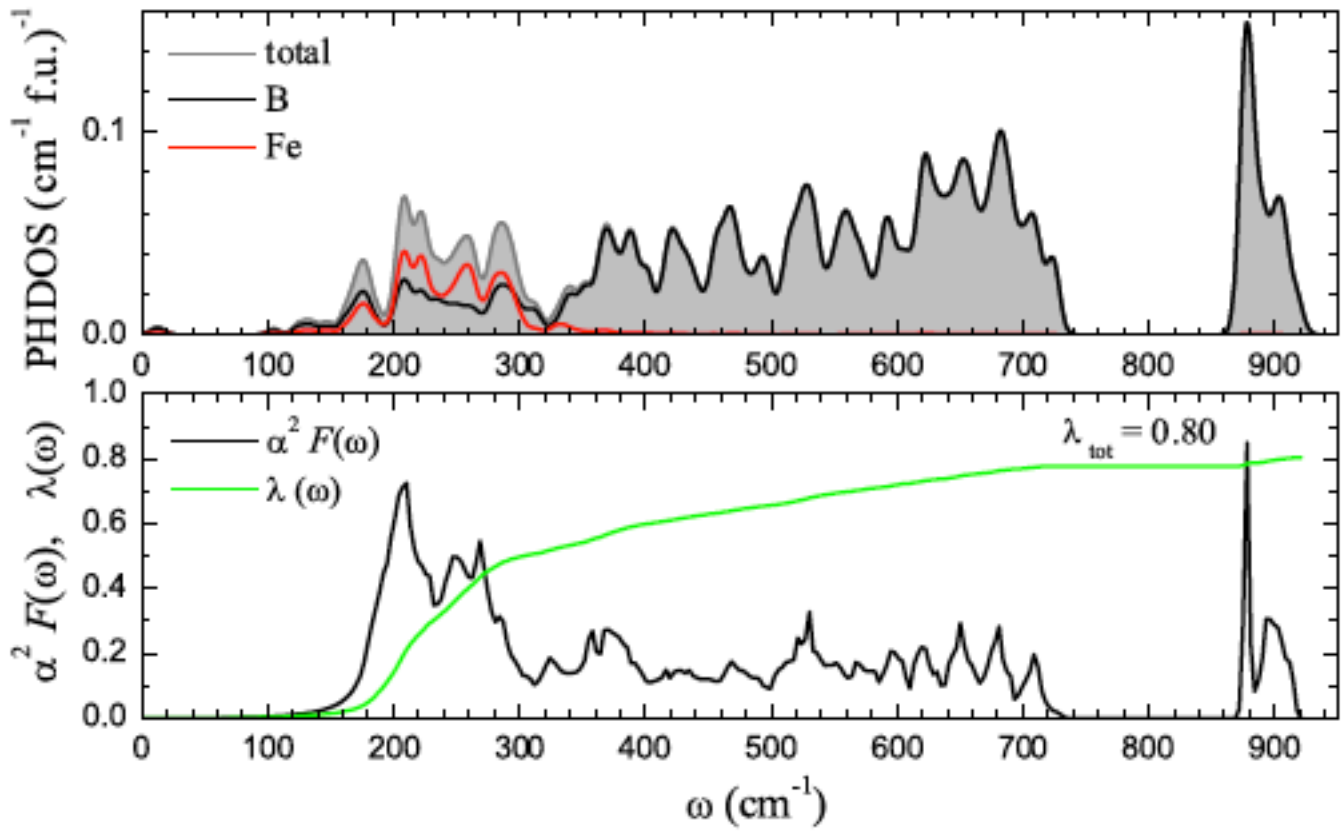
oI10-FeB_4
oP10-FeB_4 (new)

oP6-FeB_2
hP6-FeB_2
oP12-FeB_2 (new)

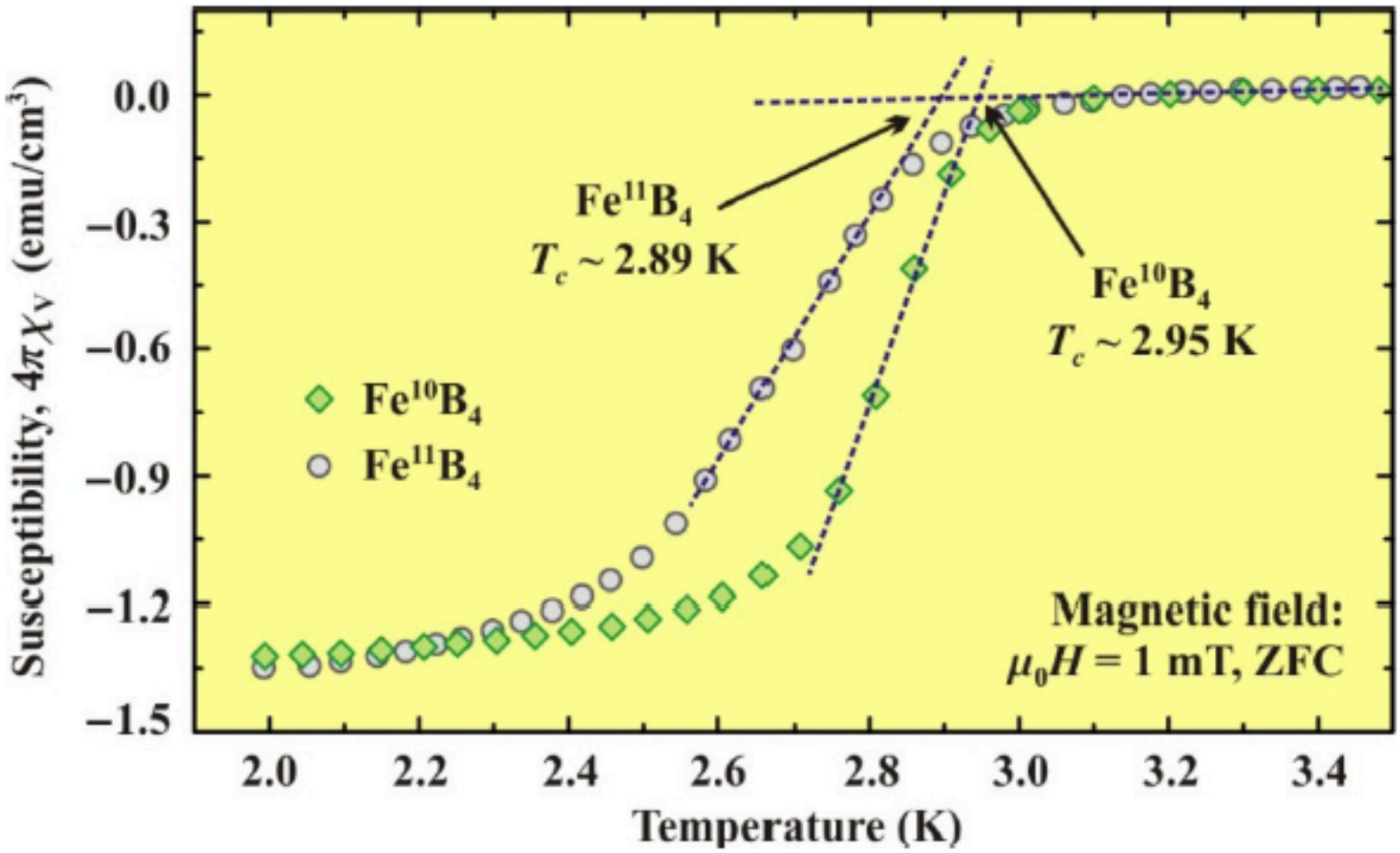
oP8-FeB
oS8-FeB
tI16-FeB

Kolmorgorov *et al*, PRL 105, 217003 (2010)

Predicted Superconductivity in *oP*10-FeB_4 (15-20K)

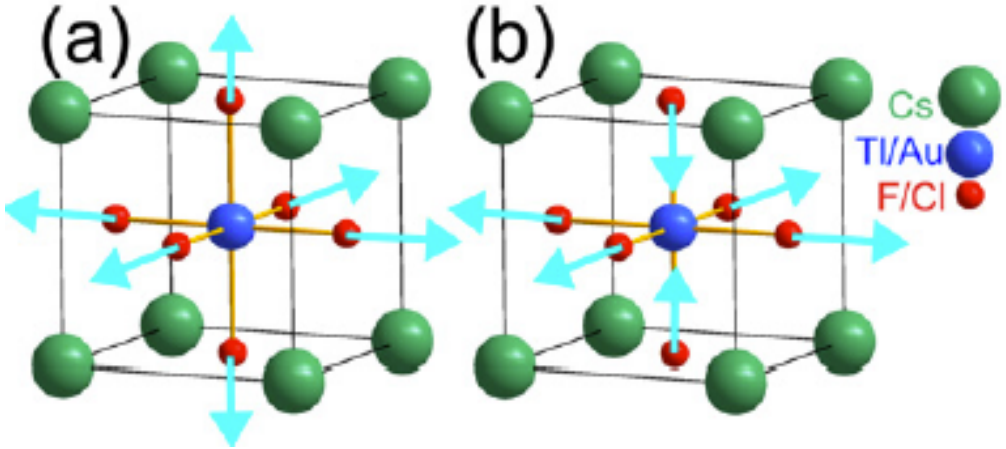


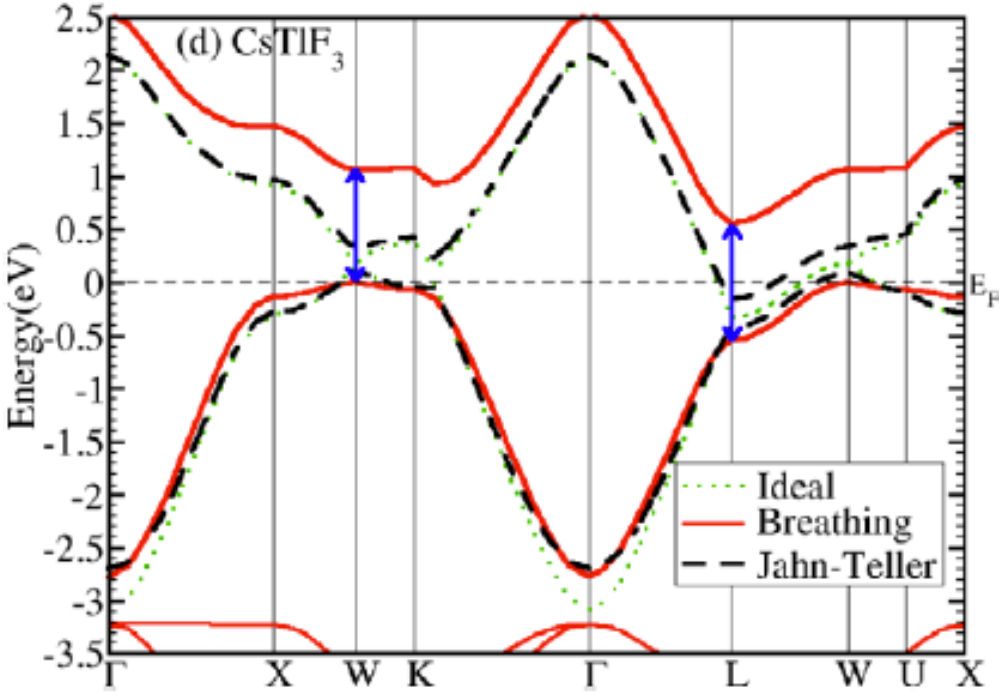
Synthesized and found to have a T_c of 3K

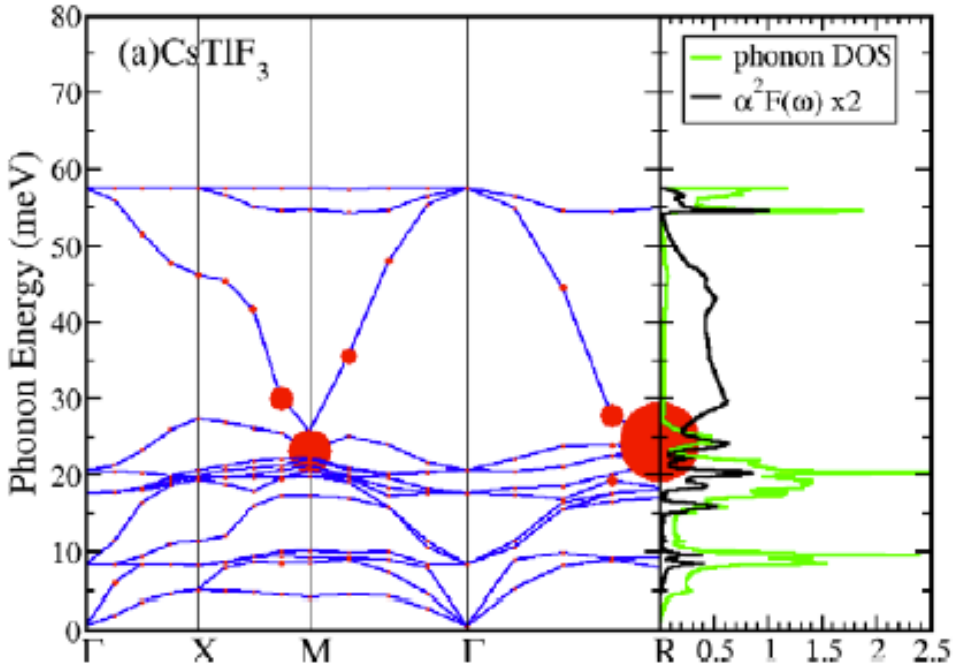


Gou *et al*, PRL 111, 157002 (2013)

Rational Materials Design based on $BaBiO_3$ ($CsTlF_3$ & $CsTlCl_3$)

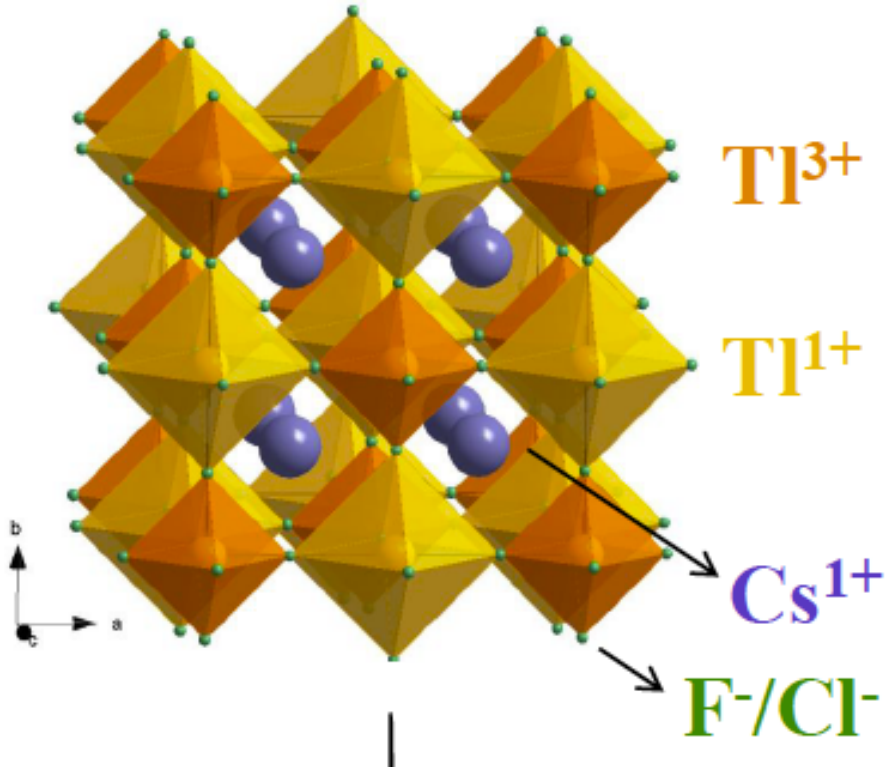


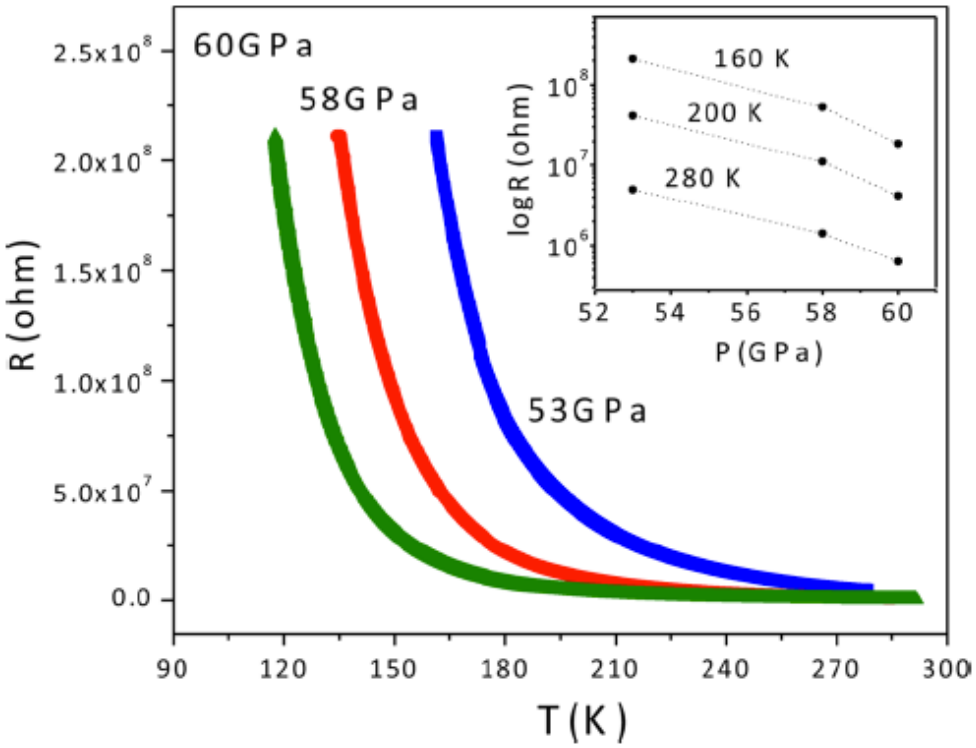




Yin & Kotliar, EPL 101, 27002 (2013)

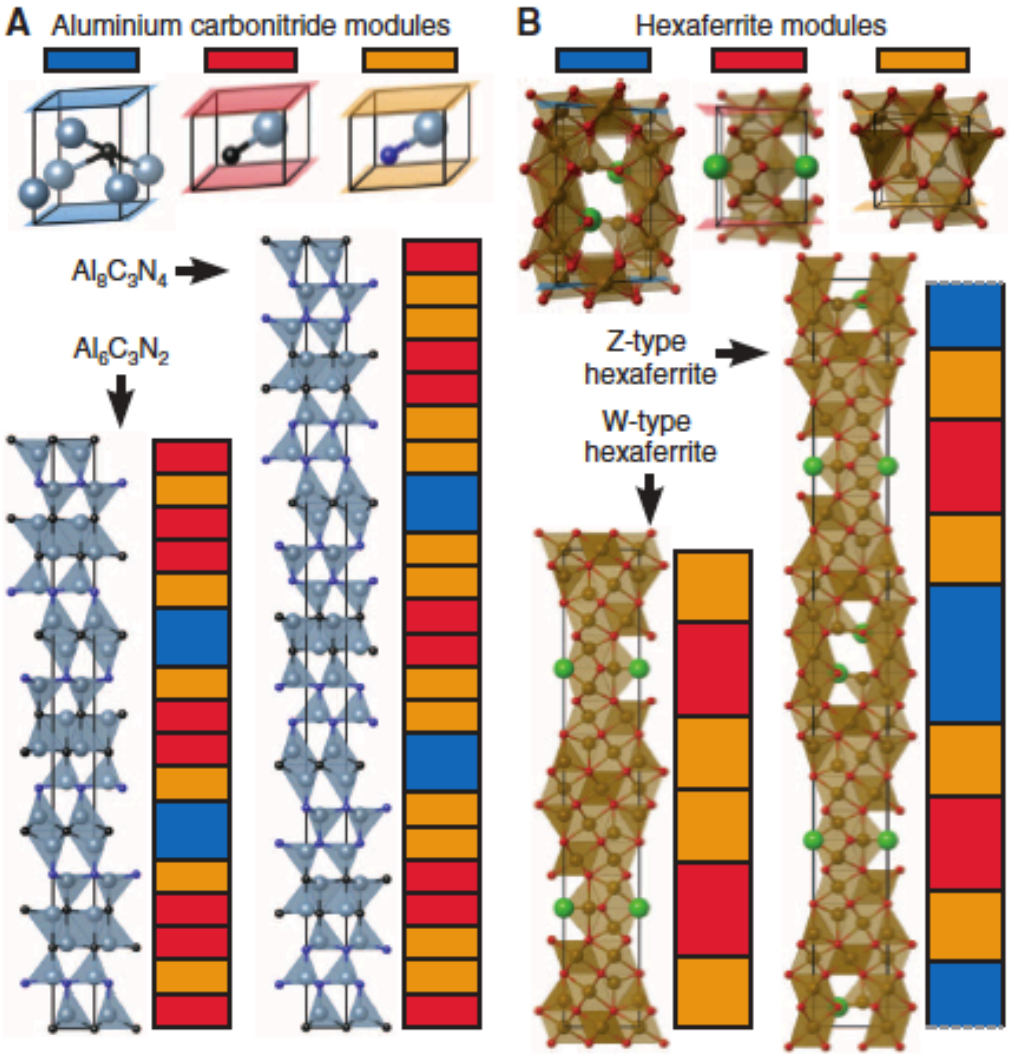
Synthesized, but samples are insulating, even at high pressures (have yet to be doped, though)

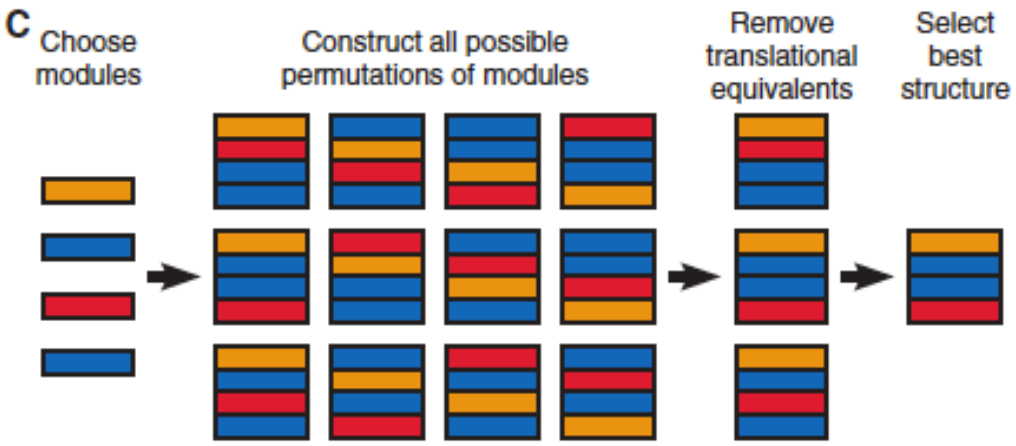


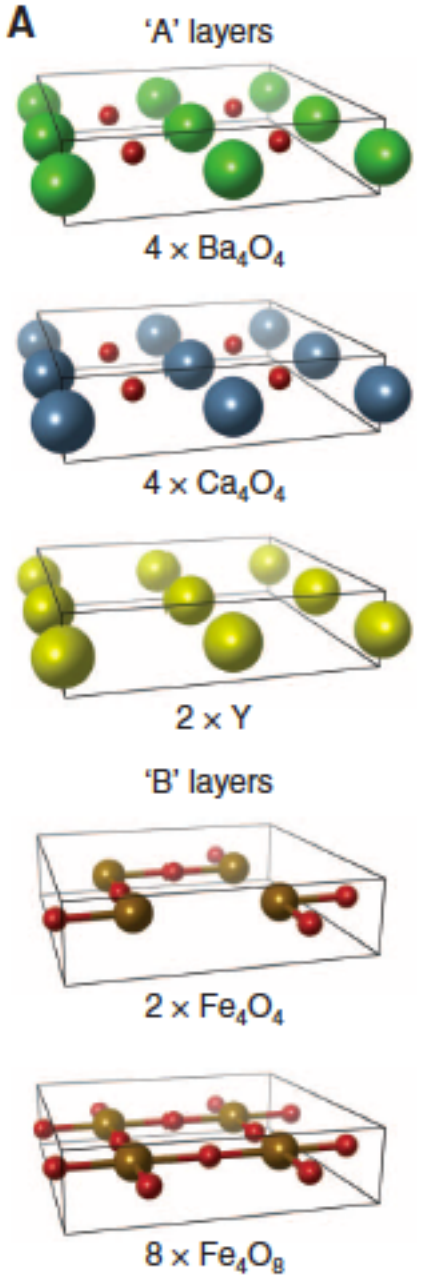


Retuerto *et al*, Chem. Mater. 25, 4071 (2013)

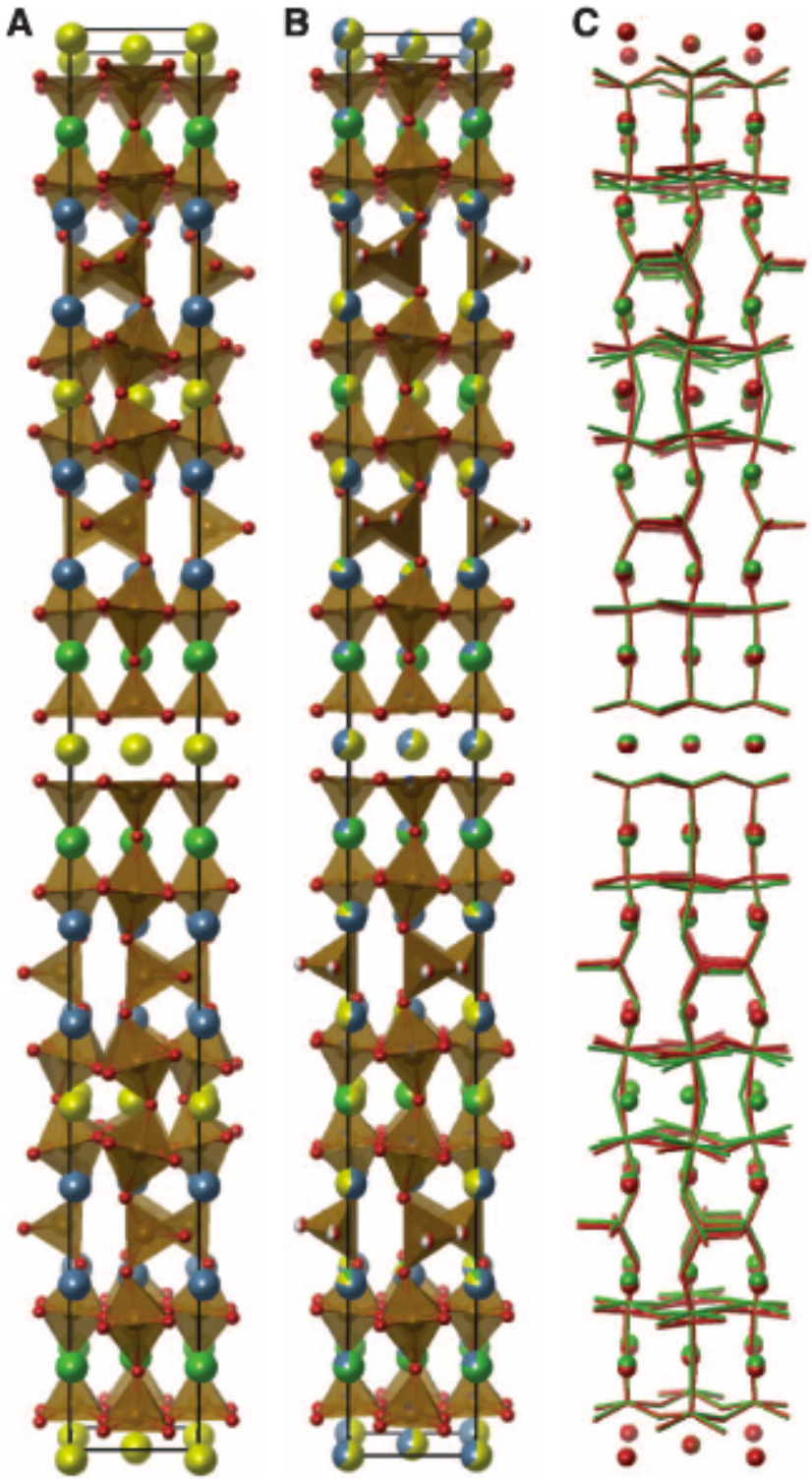
Modular Construction





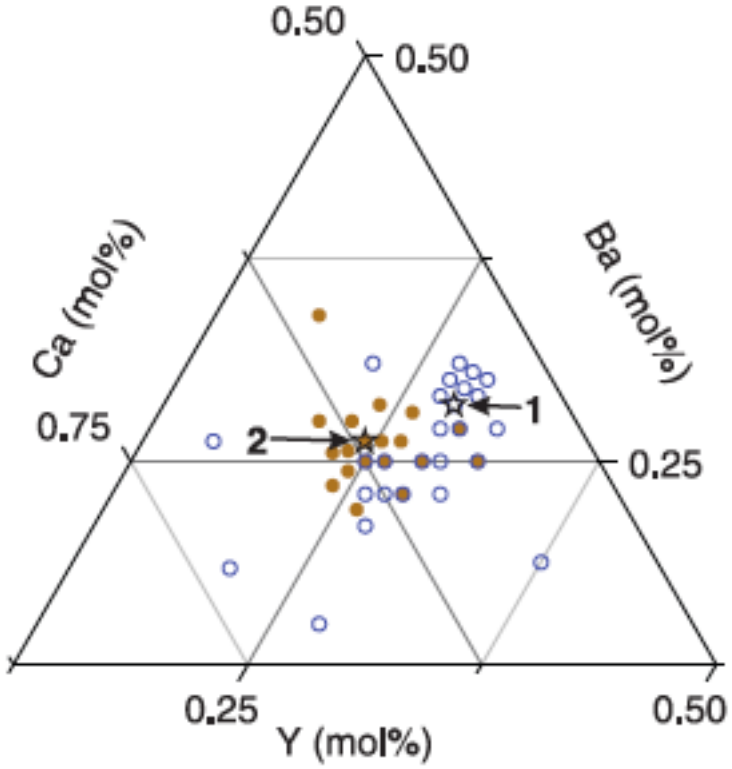


Dyer *et al*, Science 340, 847 (2013)



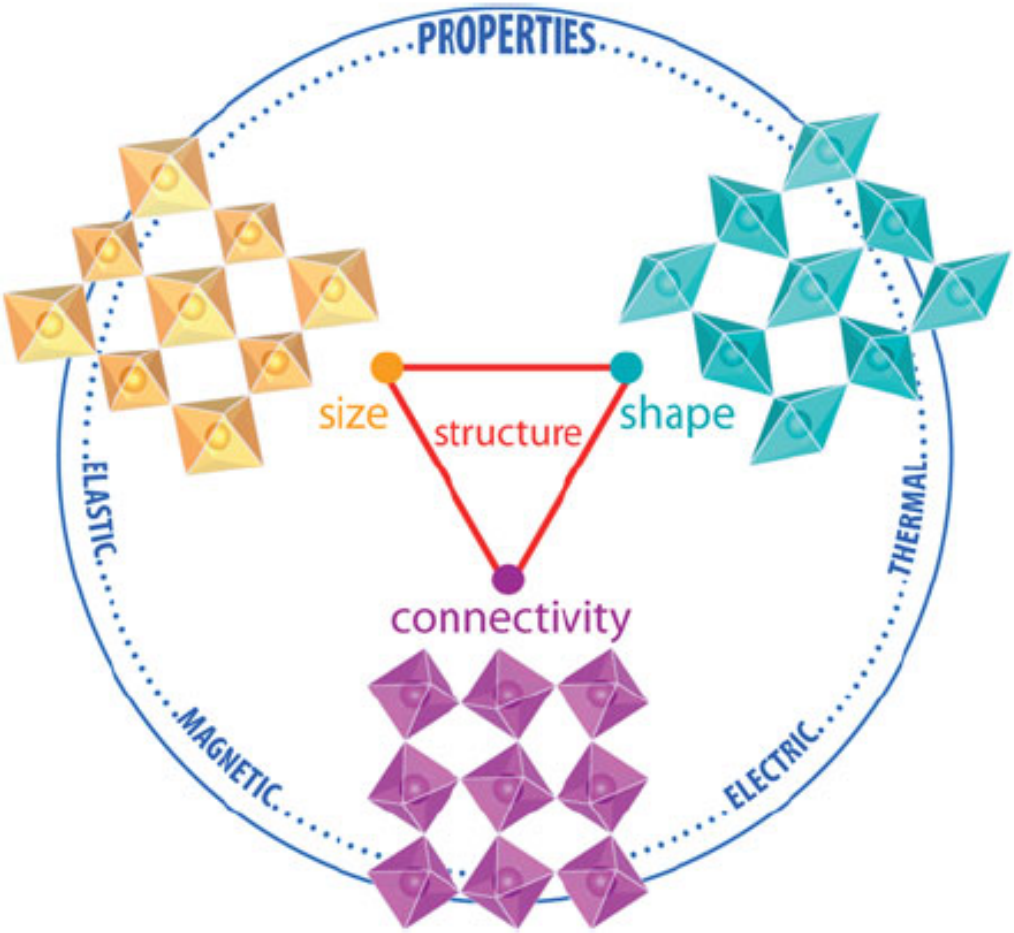
$Y_{2.24}Ba_{2.28}Ca_{3.48}Fe_{7.44}Cu_{0.56}O_{21}$

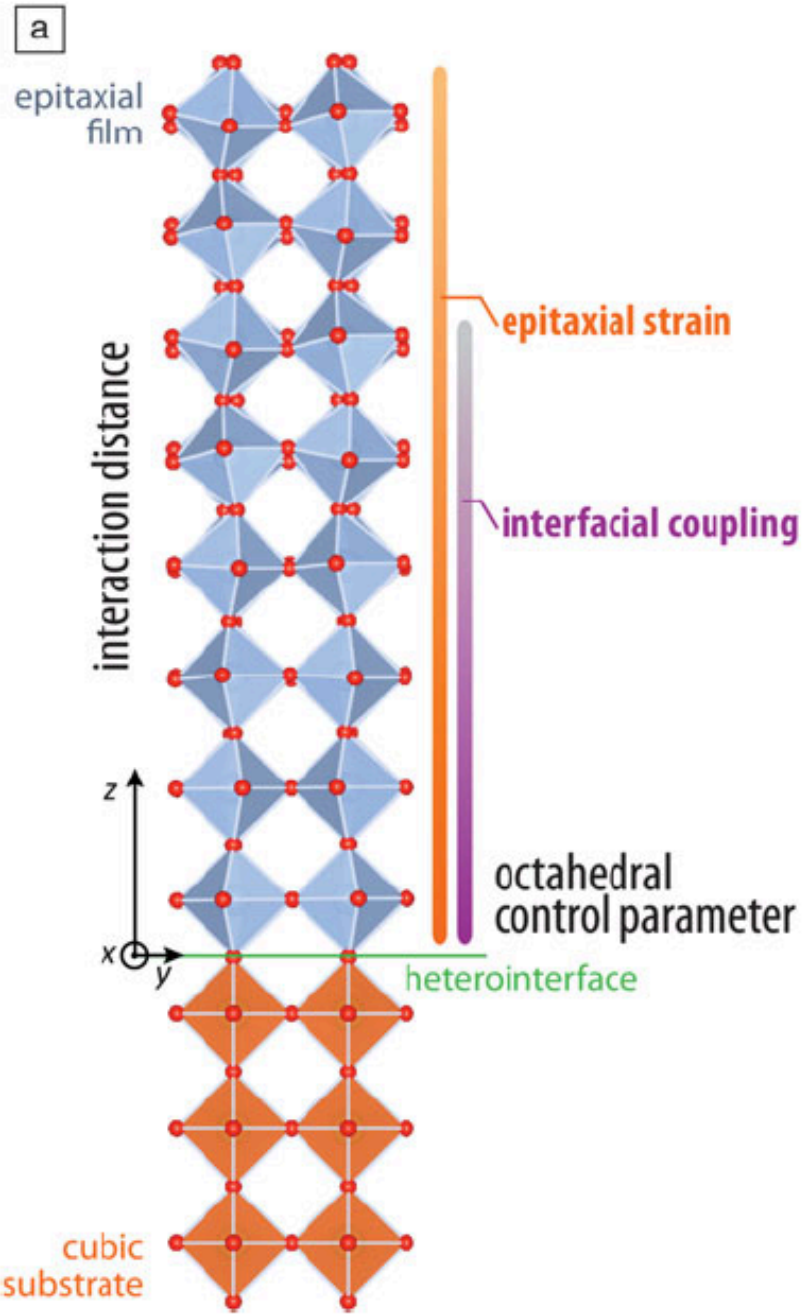
(iron analogue of Bi2212)



Predicted structure close to synthesized one

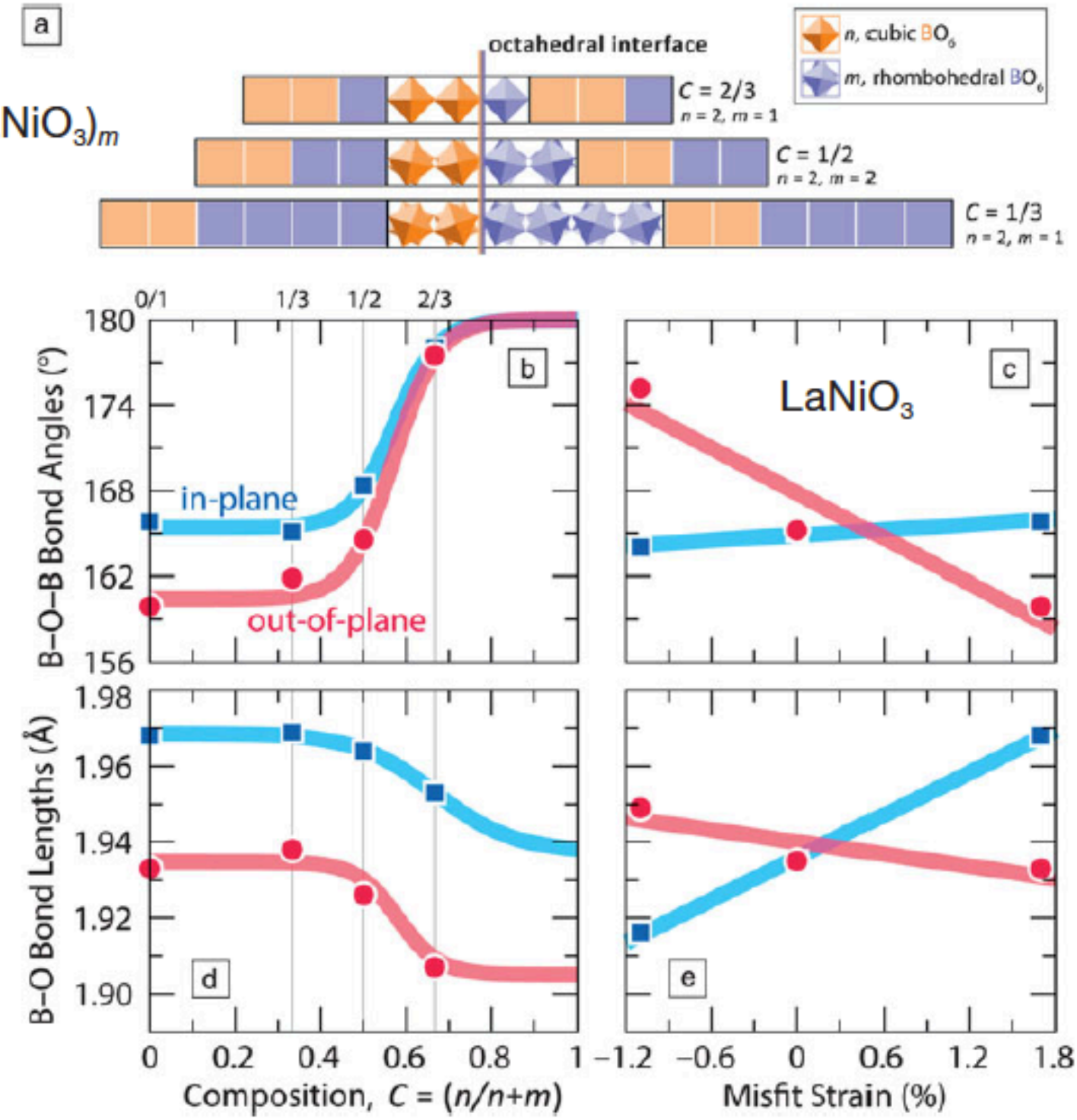
Octahedral Engineering





Rondinelli, May & Freeland,
MRS Bulletin 37, 261 (2012)

$(SrMnO_3)_n/(LaNiO_3)_m$



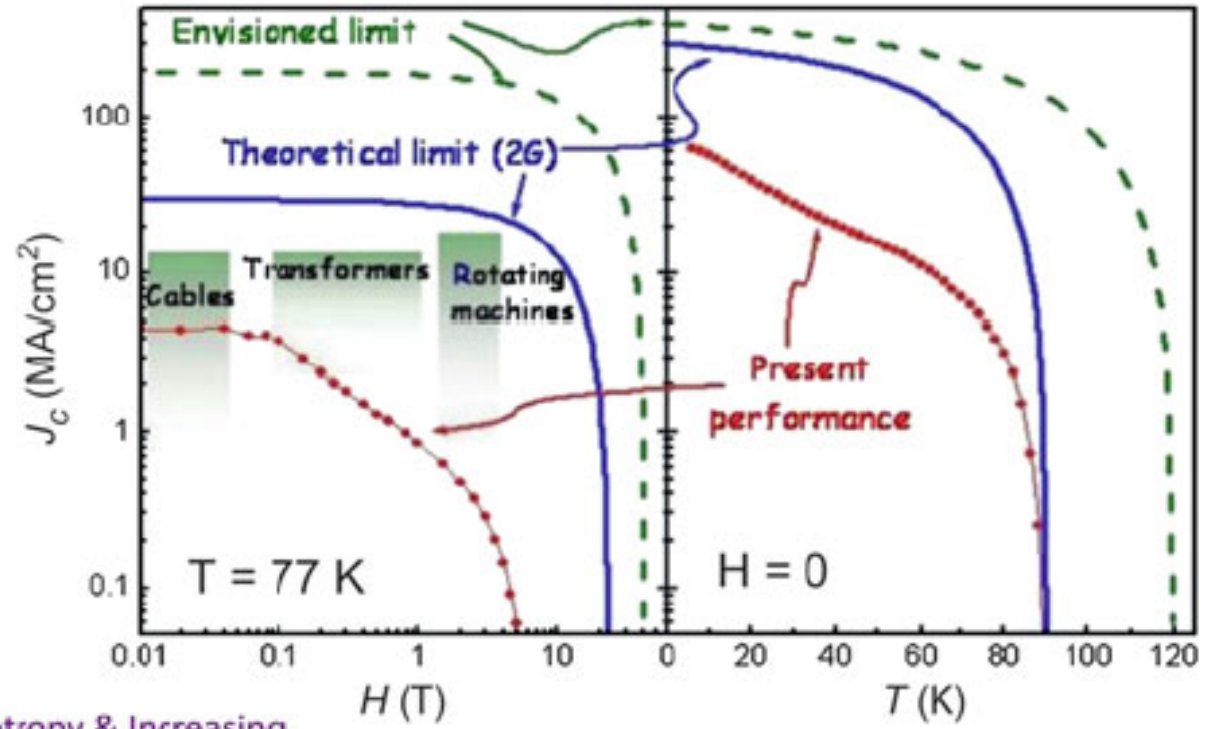
An increased T_c leads to a reduced phase stiffness

$$\frac{T_\phi}{T_p} \propto \frac{n_s^* v_F}{\gamma T_p^2}$$

$$T_c = \min\{T_\phi, T_p\}$$

$$J_c \propto n_s^* T_p$$

$$\gamma = \sqrt{\frac{M}{m}}$$



Decreasing Anisotropy & Increasing Pair Density (Cumulative)

Increasing Pairing Interaction - T_p

T_p	T_c $\frac{J_c}{J_c^{YBCO}}$	$\gamma \to 1$	n_s^* x 2	n_s^* x 10
90 K (YBCO)	90 K 1	90 K 1	90 K 2	90 K 10
180 K	72 K 2	180 K 2	180 K 4	180 K 20
270 K	54 K 3	270 K 3	270 K 6	270 K 30
360 K	36 K 4	180 K 4	360 K 8	360 K 40

Beasley, MRS Bulletin (2011)

I leave you with some “infamous” Bernd Matthias quotes:

I also want to begin with a friendly introduction because the rest of my talk will not be so friendly – *1969 Spring Superconducting Symposium (NRL, 1969)*

The electron-phonon interaction always reminds me of the man who is looking for his keys under a street light and his friends say “but you didn’t lose them here, you lost your keys over there”. “I know, but it is too dark over there.”

this reminds me of the Virginia Wolf play where four people argue all night about the aberrations of a child, and when the play is over, it turns out that there never was a child. This is exactly how I feel about the organic superconductors.

That of course leads you to Green’s functions and the absence of any further predictions. – *Science and Technology of Superconductivity (Plenum, 1973)*

Unless we accept this fact and submit to a dose of reality, honest and not so honest speculations will persist until all that is left in this field will be these scientific opium addicts, dreaming and reading one another’s absurdities in a blue haze. - *Comments Solid State Physics, 3, 93 (1970)*